

High-Throughput Identification of Electrides from all Known Inorganic Materials

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Herein, the structures and band diagrams for the full list of 69 candidate electrides are displayed in order of the Materials Project materials ID number. Red and blue colour of the bands is used to indicate spin up/down energies, where band splitting can be indicative of magnetism. The chemical formula, crystal type and symmetry are also included, along with origin of the structure information (e.g. ICSD etc). Using the structure_matcher functionality of the pymatgen analysis module the structures are grouped together by nominal compound ‘type’ nomenclature, for example “CrB-type”. We scale back the isosurface to find an ‘origin’ of the anionic electron and construct a coordinate environment for each case from this. Finally, the convergence of quasi-particle energy corrections is included at the end of the document.

Materials Project ID	Formula	Energy above hull (meV/atom)	Providence	System	Symmetry (Hermann–Mauguin notation)	Symmetry number	Electride type
mp-10045	Ba ₅ As ₃	8.5	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-10961	La ₅ Si ₃	0	ICSD	tetragonal	I4/mcm	140	0D
mp-11404	PrGa	0	ICSD	orthorhombic	Cmcm	63	2D
mp-11840	BaAg	0	ICSD	orthorhombic	Pnma	62	0D
mp-12467	Ca ₅ Sb ₃	0.80	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-12612	Ba ₃ Ag ₂	0.54	ICSD	trigonal	R-3	148	0D
mp-12723	CaAu	0	ICSD	orthorhombic	Cmcm	63	2D
mp-12905	Ba ₃ CrN ₃	0	ICSD	hexagonal	P6 ₃ /m	176	1D
mp-12906	Sr ₃ CrN ₃	0	ICSD	hexagonal	P6 ₃ /m	176	1D
mp-13053	SrSi	7.4	ICSD	orthorhombic	Pnma	62	0D
mp-1334	Y ₂ C	0	ICSD	trigonal	R-3m	166	2D
mp-1363	Na ₂ Au	0	ICSD	tetragonal	I4/mcm	140	1D
mp-1448	NdGa	0	ICSD	orthorhombic	Cmcm	63	2D
mp-1464	Nd ₅ Ge ₃	0	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-1563	CaSi	0	ICSD	orthorhombic	Cmcm	63	2D
mp-15698	Sr ₅ As ₃	0	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-1698	SrSn	0	ICSD	orthorhombic	Cmcm	63	2D
mp-1730	BaGe	0	ICSD	orthorhombic	Cmcm	63	2D
mp-17325	Ba ₅ Sn ₃	9.2	ICSD	tetragonal	I4/mcm	140	0D
mp-17720	Sr ₅ Sn ₃	3.0	ICSD	tetragonal	I4/mcm	140	0D
mp-17757	Sr ₅ Ge ₃	2.5	ICSD	tetragonal	I4/mcm	140	0D
mp-18167	Ca ₃ Cd ₂	0	ICSD	tetragonal	P4 ₂ /mnm	136	0D
mp-18316	Mg ₂ Pd	0	ICSD	cubic	Fd-3m	227	0D
mp-1884	Ca ₅ Ge ₃	0	ICSD	tetragonal	I4/mcm	140	0D
mp-20909	La ₃ In	0	ICSD	cubic	Pm-3m	221	0D
mp-2147	SrGe	0	ICSD	orthorhombic	Cmcm	63	2D
mp-21483	Nd ₃ In	0	ICSD	cubic	Pm-3m	221	0D
mp-2360	CaGe	0	ICSD	orthorhombic	Cmcm	63	2D
mp-24153	LaH ₂	0	ICSD	cubic	Fm-3m	225	0D
mp-2499	BaSi	0	ICSD	orthorhombic	Cmcm	63	2D
mp-2538	Y ₅ Si ₃	0	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-2585	Sr ₅ Sb ₃	0	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-2631	Ba ₄ Al ₅	0	ICSD	hexagonal	P6 ₃ /mmc	194	0D
mp-2661	SrSi	0	ICSD	orthorhombic	Cmcm	63	2D
mp-2686	Ca ₂ N	0	ICSD	trigonal	R-3m	166	2D
mp-28489	Ca ₅ (GaN ₂) ₂	0	ICSD	orthorhombic	Cmca	64	0D
mp-29620	Sr ₅ Bi ₃	0	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-29621	Ba ₅ Bi ₃	0	ICSD	hexagonal	P6 ₃ /mcm	193	1D
mp-30355	SrAg	0	ICSD	orthorhombic	Pnma	62	0D
mp-30357	Sr ₃ Ag ₂	0	ICSD	trigonal	R-3	148	0D
mp-30366	Ca ₃ Au	0	ICSD	orthorhombic	Pnma	62	0D
mp-30367	Ca ₅ Au ₂	0	ICSD	monoclinic	C2/c	15	0D
mp-30368	Ca ₅ Au ₃	0	ICSD	tetragonal	I4/mcm	140	0D

mp-30422	Sr ₇ Au ₃	0	ICSD	hexagonal	P6 3mc	186	1D
mp-371	La ₃ Tl	0	ICSD	cubic	Pm-3m	221	0D
mp-4579	LaSiRu	0	ICSD	tetragonal	P4/nmm	129	2D
mp-4738	PrScGe	0	ICSD	tetragonal	I4/mmm	139	2D
mp-4854	NdScGe	0	ICSD	tetragonal	I4/mmm	139	2D
mp-542680	Na ₃ In ₂ Au	0	ICSD	cubic	Fd-3m	227	0D
mp-542681	Na ₃ In ₂ Ag	0	ICSD	cubic	Fd-3m	227	0D
mp-567342	Nd ₄ MgIr	0	ICSD	cubic	F-43m	216	0D
mp-569535	Ca ₂ Bi	0	ICSD	tetragonal	I4/mmm	139	0D
mp-570400	Ba ₇ Al ₁₀	0	ICSD	trigonal	R-3m	166	0D
mp-573908	Sr ₁₁ (MgSi ₅) ₂	6.1	ICSD	monoclinic	C2/m	12	0D
mp-605873	Pr ₄ MgRu	0	ICSD	cubic	F-43m	216	0D
mp-630923	Ba ₃ Pb ₅	0	ICSD	orthorhombic	Cmcm	63	0D
mp-645130	Pr ₄ MgCo	0	ICSD	cubic	F-43m	216	0D
mp-693	Pr ₃ Tl	3.8	ICSD	cubic	Pm-3m	221	0D
mp-7376	Sr ₃ (AlSn) ₂	0	ICSD	orthorhombic	Immm	71	0D
mp-746	Sr ₅ Si ₃	0	ICSD	tetragonal	I4/mcm	140	0D
mp-7507	Sr ₃ Li ₂	0	ICSD	tetragonal	P4 2/mnm	136	0D
mp-793	Ca ₅ Si ₃	0	ICSD	tetragonal	I4/mcm	140	0D
mp-8320	SmScSi	0	ICSD	tetragonal	I4/mmm	139	2D
mp-872	BaSn	0	ICSD	orthorhombic	Cmcm	63	2D
mp-973508	KRb ₃	6.3	OQMD	tetragonal	I4/mmm	139	0D
mp-974066	Nd ₃ Sm	8.9	OQMD	cubic	Pm-3m	221	0D
mp-976115	K ₃ Rb	5.2	OQMD	hexagonal	P6 3/mmc	194	0D
mp-984744	Ca ₃ Tl	3.0	OQMD	hexagonal	P6 3/mmc	194	1D
mp-9909	Ba ₅ Sb ₃	0	ICSD	hexagonal	P6 3/mcm	193	1D

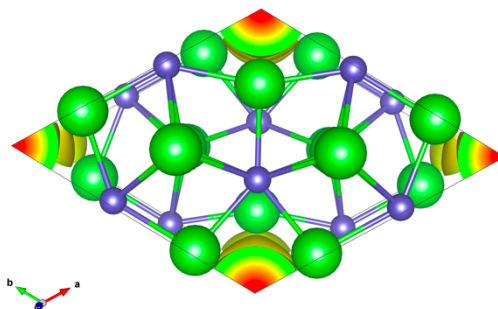
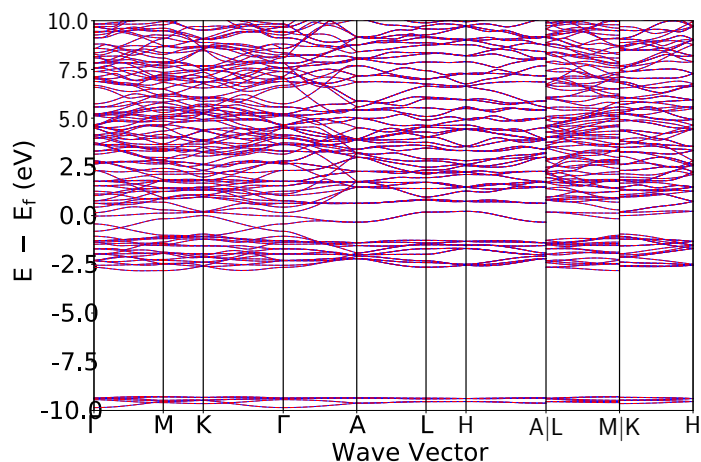


Figure 1: Ba_5As_3 (mp-10045). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD;¹ comments: referred to as intermetallic. Anionic electron coordination environment: octahedral with Ba.

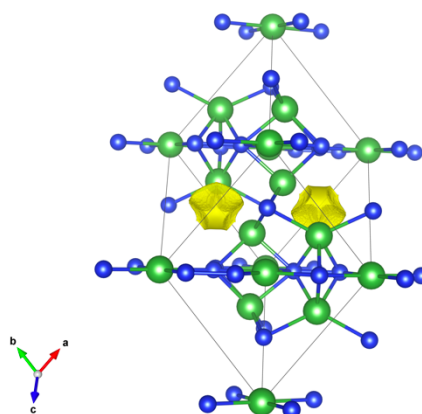
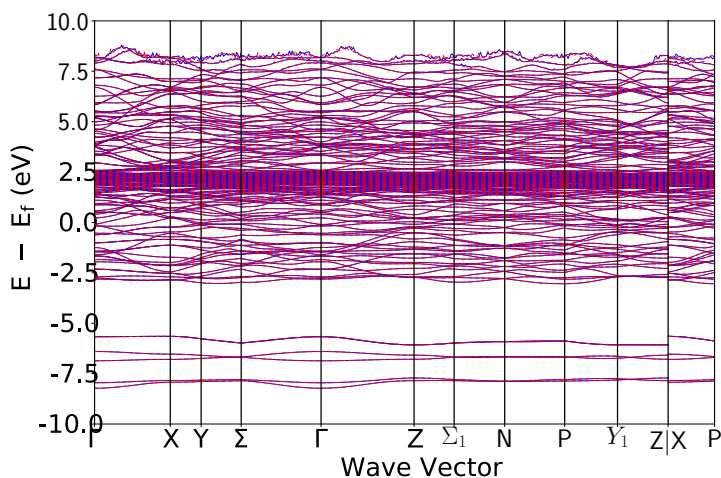


Figure 2: La_5Si_3 (mp-10961). Symmetry: tetragonal; $I4/mcm$ (number 140). Structure: Cr_5B_3 -type. Origin: ICSD;² comments: an “electronic delocalization” is observed that is proposed to be the origin of “unusual electrical resistivity” for this compound. Anionic electron coordination environment: tetrahedral with La.

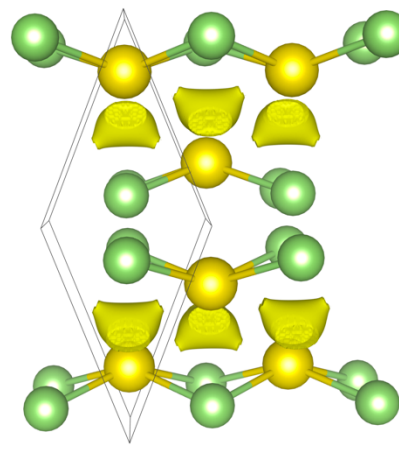
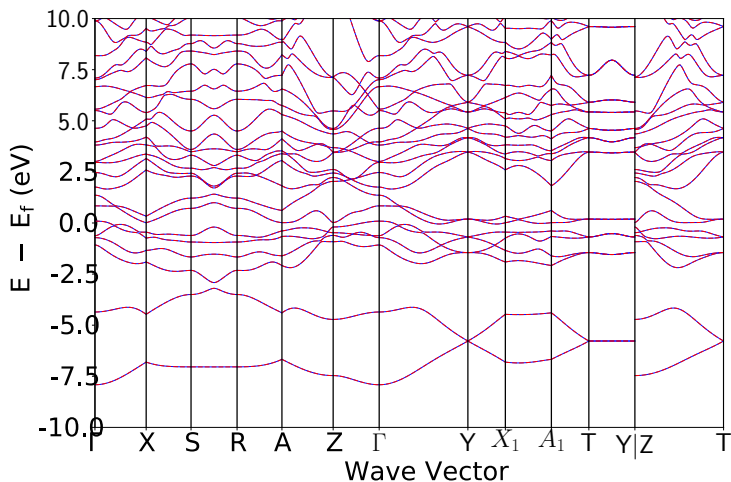


Figure 3: PrGa (mp-11404). Symmetry: orthorhombic; $Cmcm$ (number 63). Structure: CrB -type. Origin: ICSD;³ comments: referred to as intermetallic. Anionic electron coordination environment: tetrahedral with Pr.

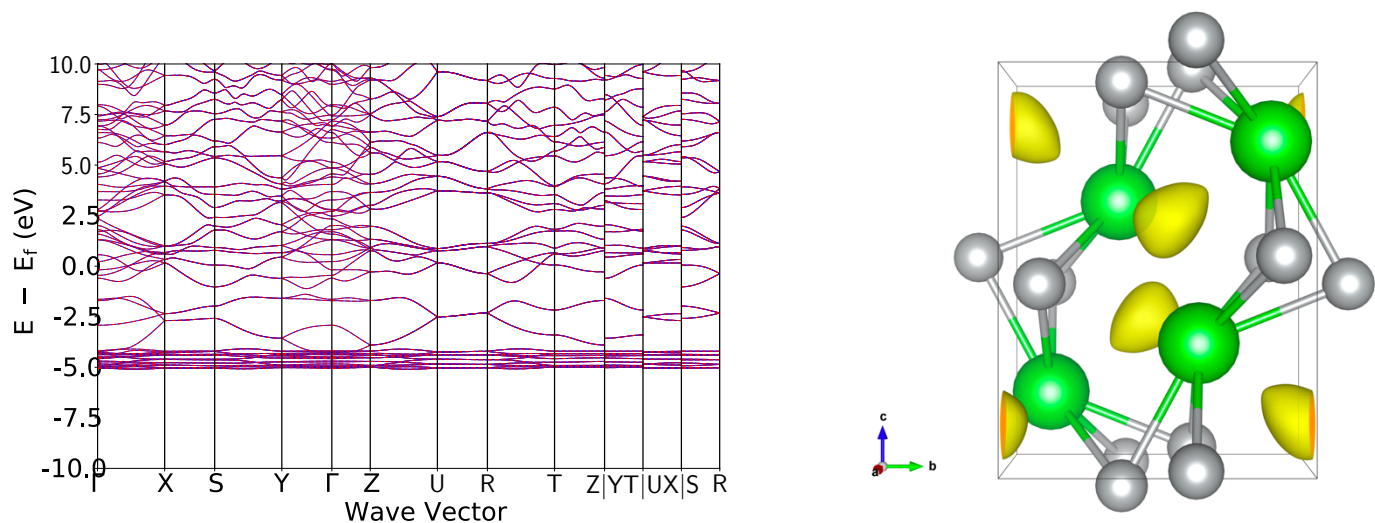


Figure 4: BaAg (mp-11840). Symmetry: Orthorhombic; Pnma (number 62). Structure: FeB-type. Origin: ICSD;⁴ comments: “The CrB and FeB types have to be considered the simplest members of a structural family based on the trigonal-prismatic coordination”. Anionic electron coordination environment: tetrahedral with Ba.

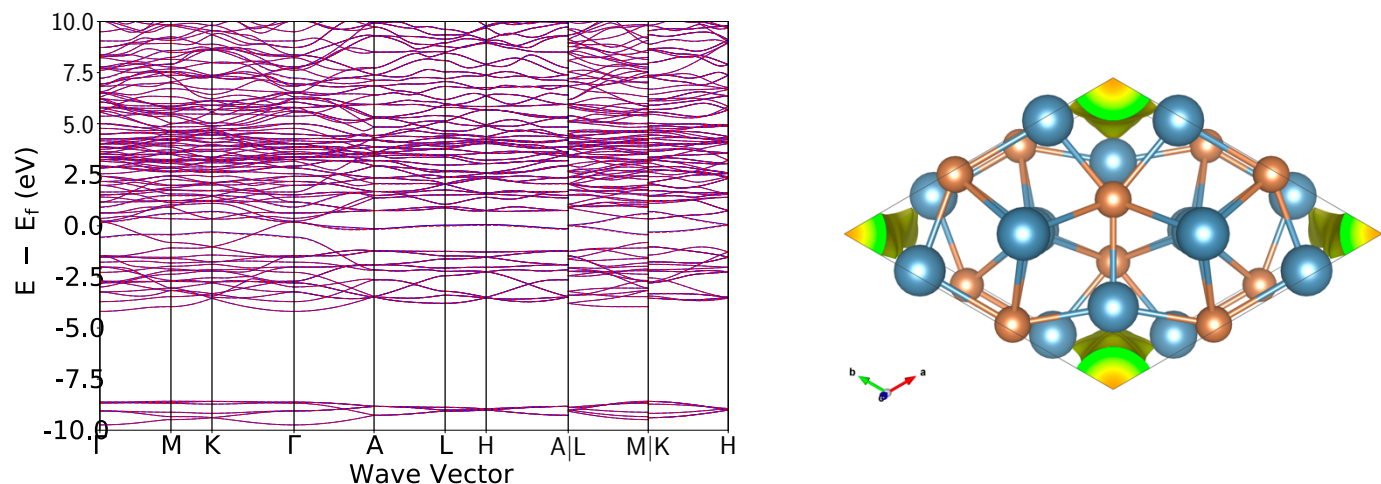


Figure 5: Ca₅Sb₃ (mp-12467). Symmetry: hexagonal; P6₃/mcm (number 193). Structure: Mn₅Si₃-type. Origin: ICSD;⁵ comments: referred to as intermetallic. Suggest previous reports of similar structures contain unresolved hydrogen within the 1-d channel of electron density. Anionic electron coordination environment: trigonal planar with Ca.

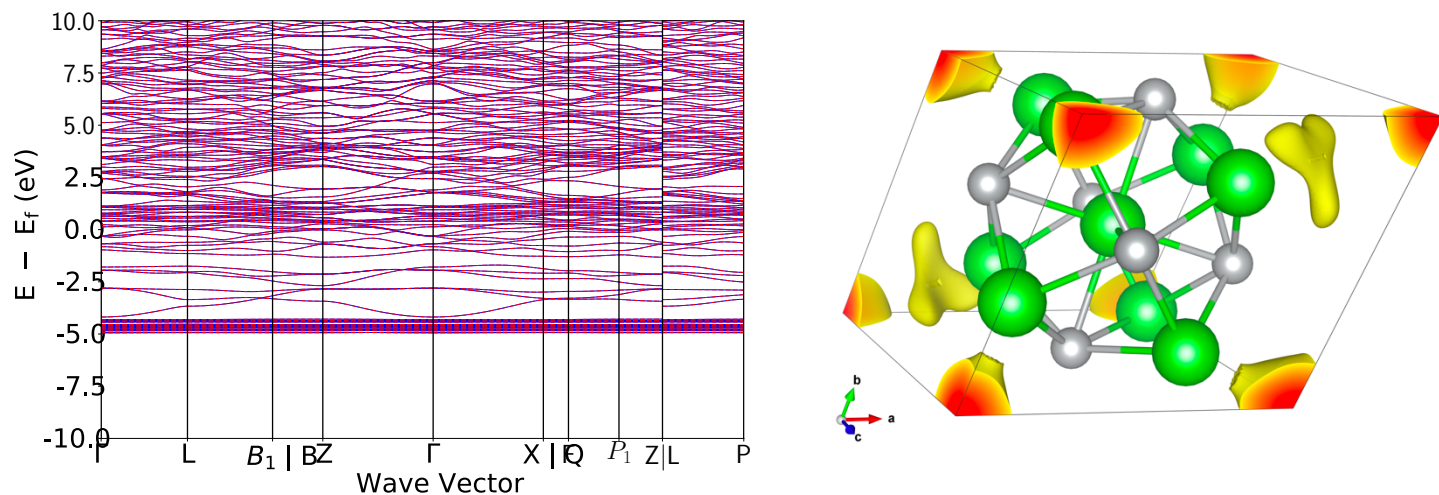


Figure 6: Ba₃Ag₂ (mp-12612). Symmetry: trigonal; R-3 (number 148). Structure: Er₃Ni₂-type. Origin: ICSD;⁶ comments: N/A. Anionic electron coordination environment: Octahedral with Ba.

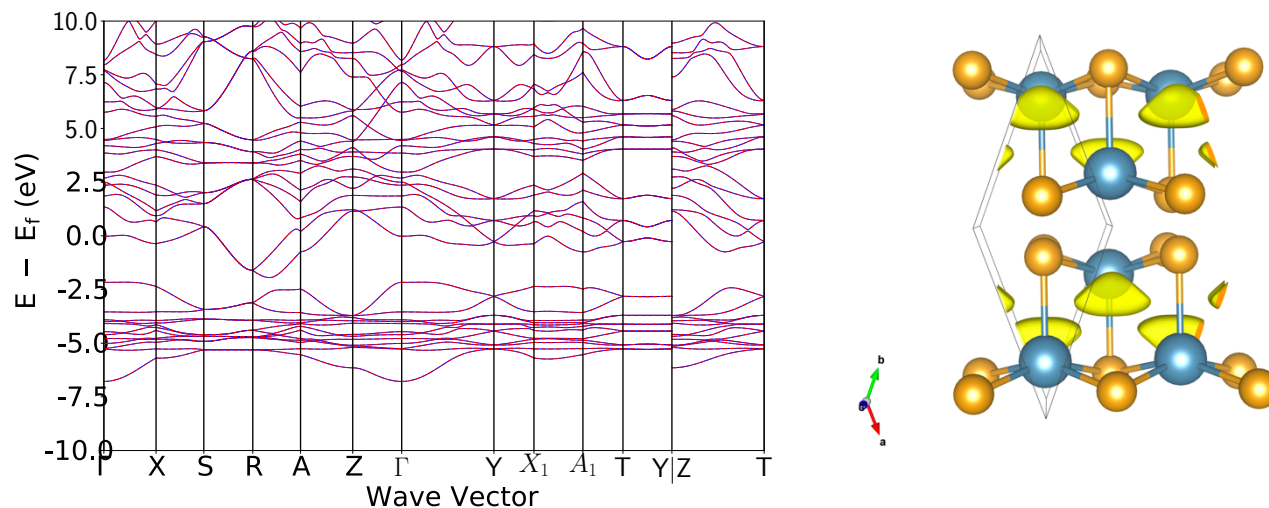


Figure 7: CaAu (mp-12723). Symmetry: orthorhombic; Cmc_m (number 63). Structure: CrB-type. Origin: ICSD;⁷ comments: N/A. Anionic electron coordination environment: distorted octahedral with Ca and Au.

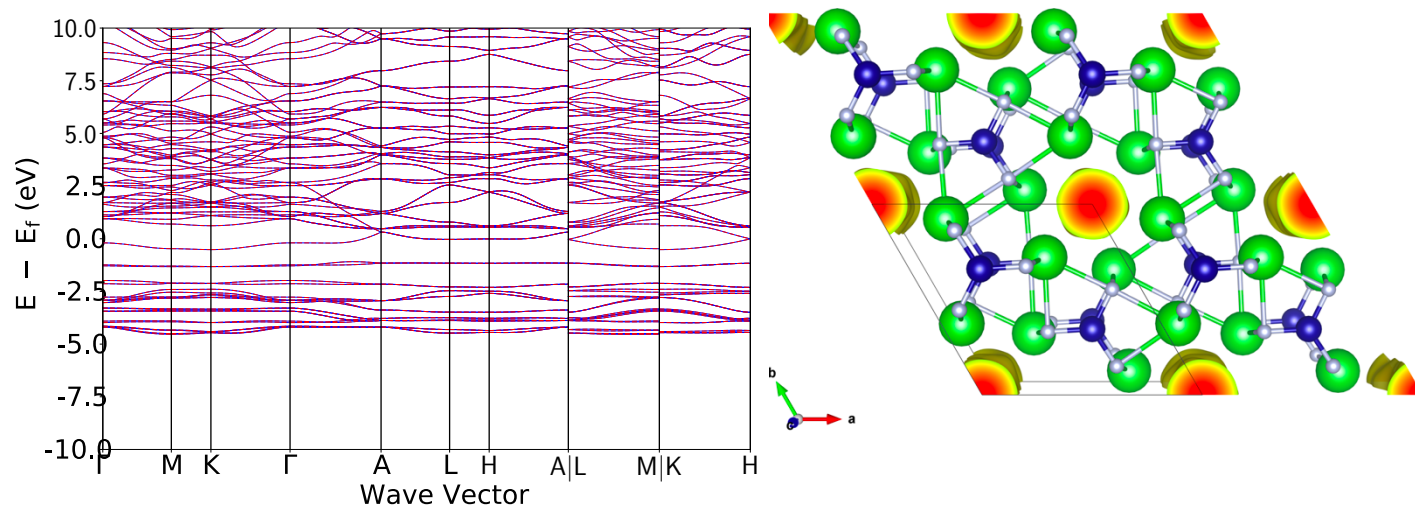


Figure 8: Ba₃CrN₃ (mp-12905). Symmetry: hexagonal; P6₃/m (number 176). Structure: Ba₃CrN₃-type. Origin: ICSD;⁸ comments: “The [calculated bond valences for Cr] deviate significantly from the expected oxidation states... and lie invariably closer to 4 than 3”. Anionic electron coordination environment: octahedral with Ba.

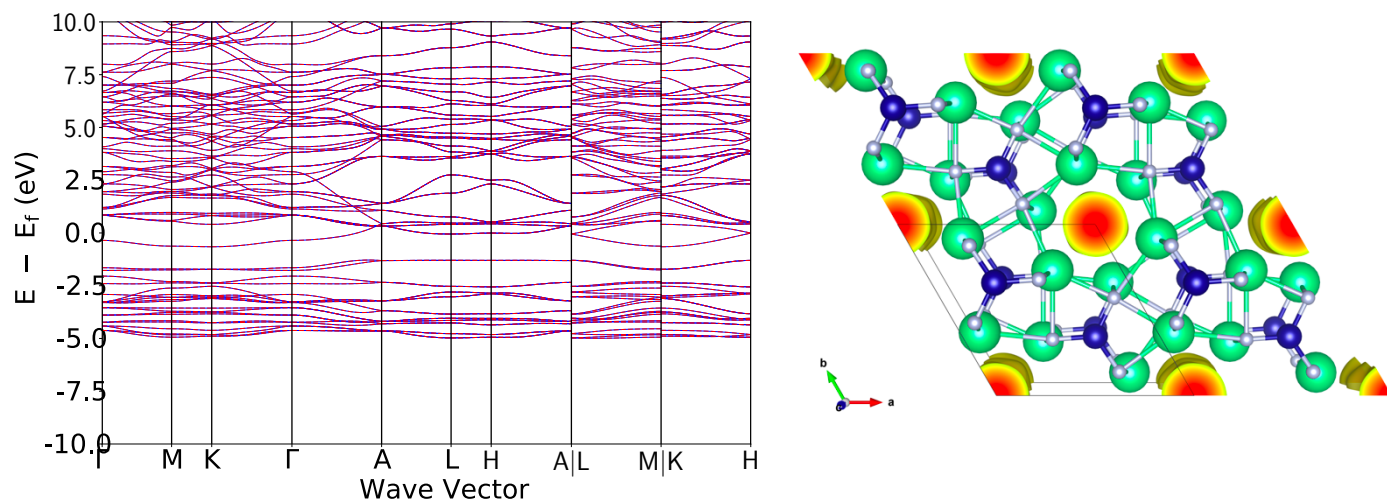


Figure 9: Sr₃CrN₃ (mp-12906). Symmetry: hexagonal; P6₃/m (number 176). Structure: Ba₃CrN₃-type. Origin: ICSD;⁸ comments: “The [calculated bond valences for Cr] deviate significantly from the expected oxidation states... and lie invariably closer to 4 than 3”. Anionic electron coordination environment: octahedral with Sr.

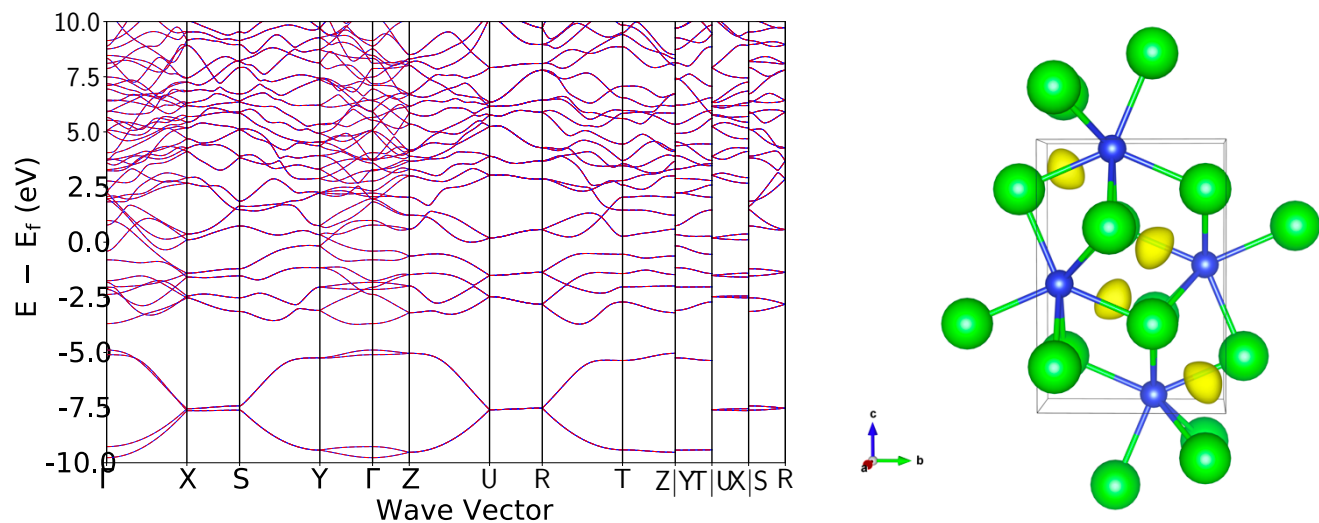


Figure 10: SrSi (mp-13053). Symmetry: Orthorhombic; Pnma (number 62). Structure: FeB-type. Origin: ICSD;⁹ *ab initio* predicted structure. Anionic electron coordination environment: distorted octahedral with Sr and Si.

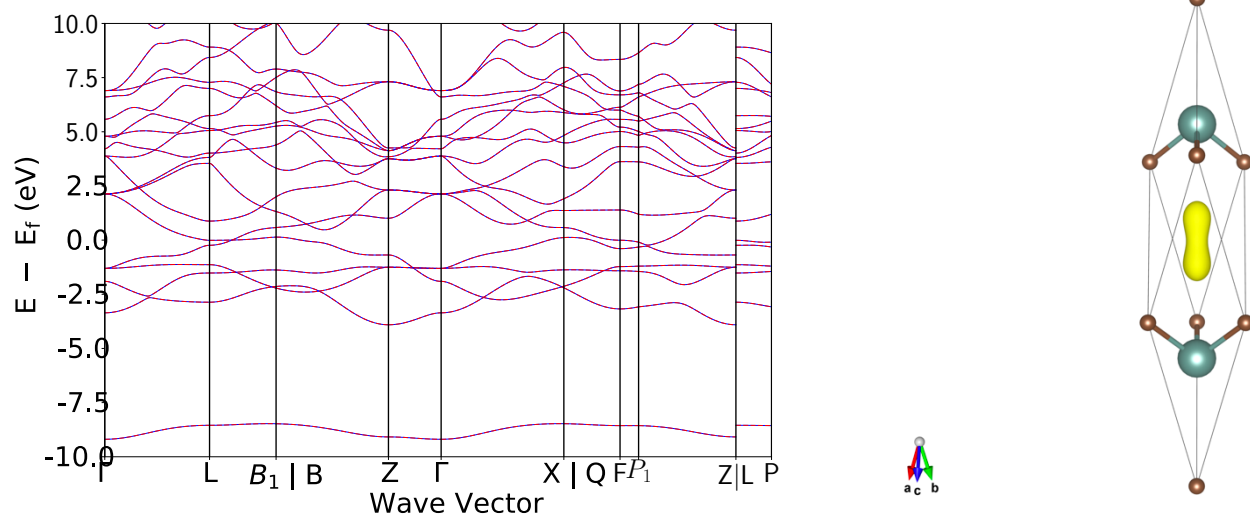


Figure 11: Y₂C (mp-1334). Symmetry: trigonal; R-3m (number 166). Structure: anti-CdCl₂-type. Origin: ICSD;¹⁰ comments: discussed Y₂C as use for hydrogen absorption. Anionic electron coordination environment: trigonal pyramidal with Y.

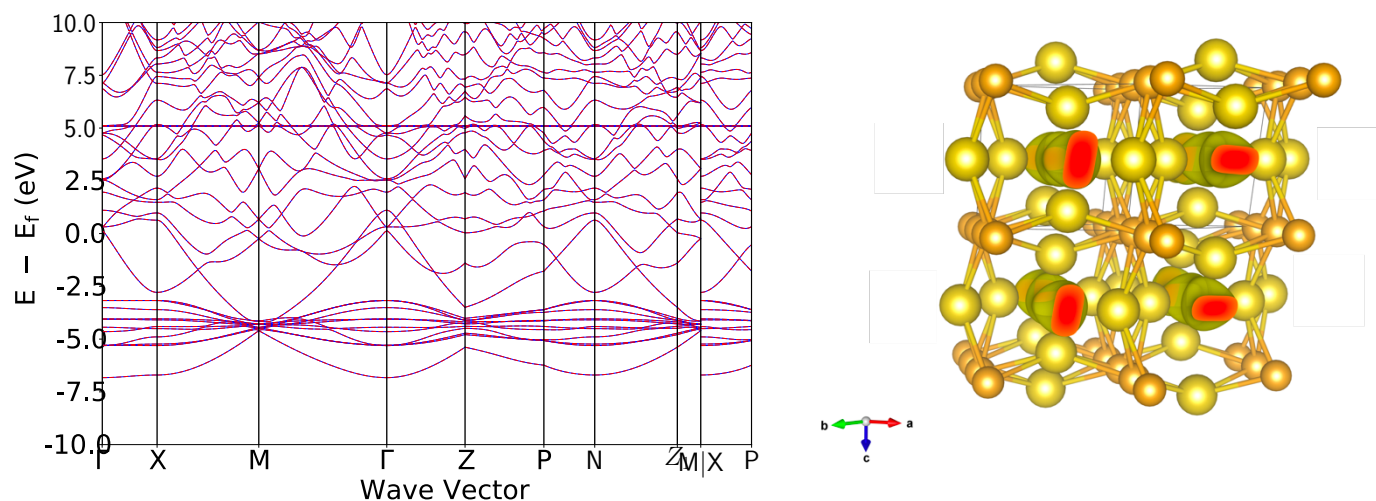


Figure 12: Na₂Au (mp-1363). Symmetry: tetragonal; I4/mcm (number 140). Structure: Cu₂Mg-type. Origin: ICSD;¹¹ comment: N/A. Anionic electron coordination environment: tetrahedral with Na.

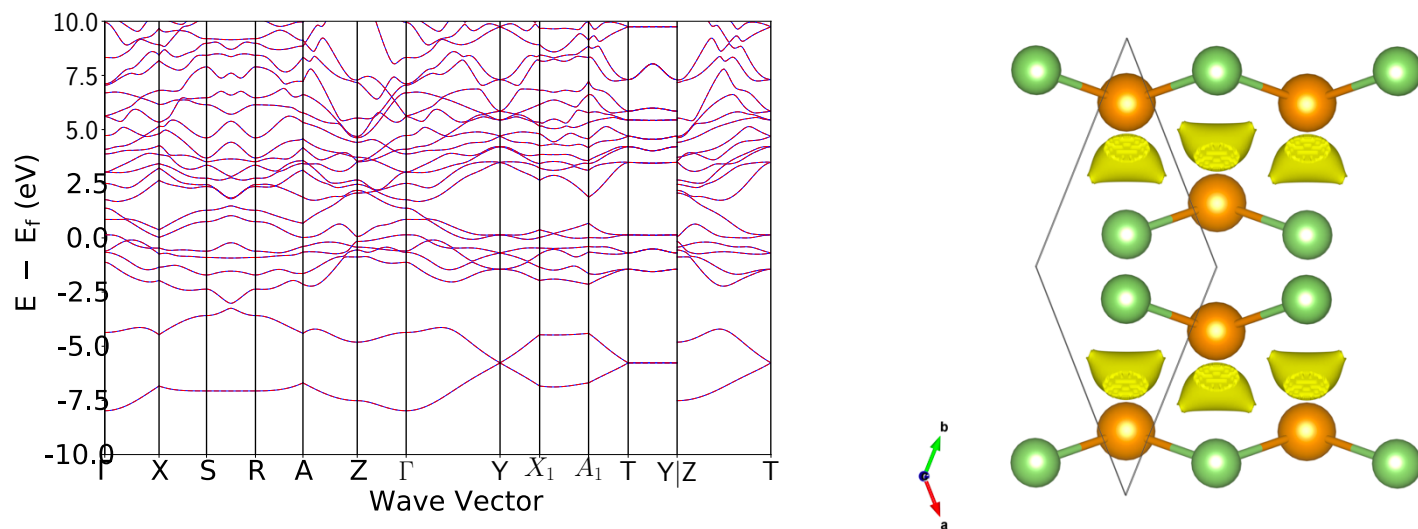


Figure 13: NdGa (mp-1448). Symmetry: orthorhombic; Cmc_m (number 63). Structure: CrB-type. Origin: ICSD;¹² comments: referred to as alloy. Anionic electron coordination environment: tetrahedral with Nd.

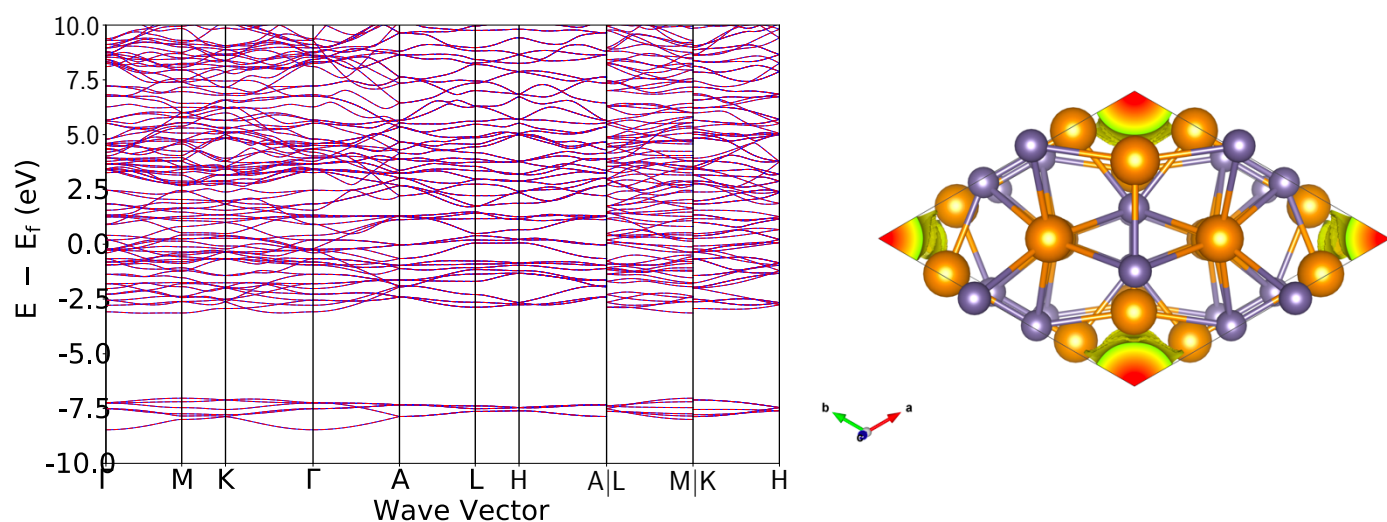


Figure 14: Nd₅Ge₃ (mp-1464). Symmetry: hexagonal; P6₃/mcm (number 193). Structure: Mn₅Si₃-type. Origin: ICSD;¹³ comments: N/A. Anionic electron coordination environment: trigonal pyramidal with Nd.

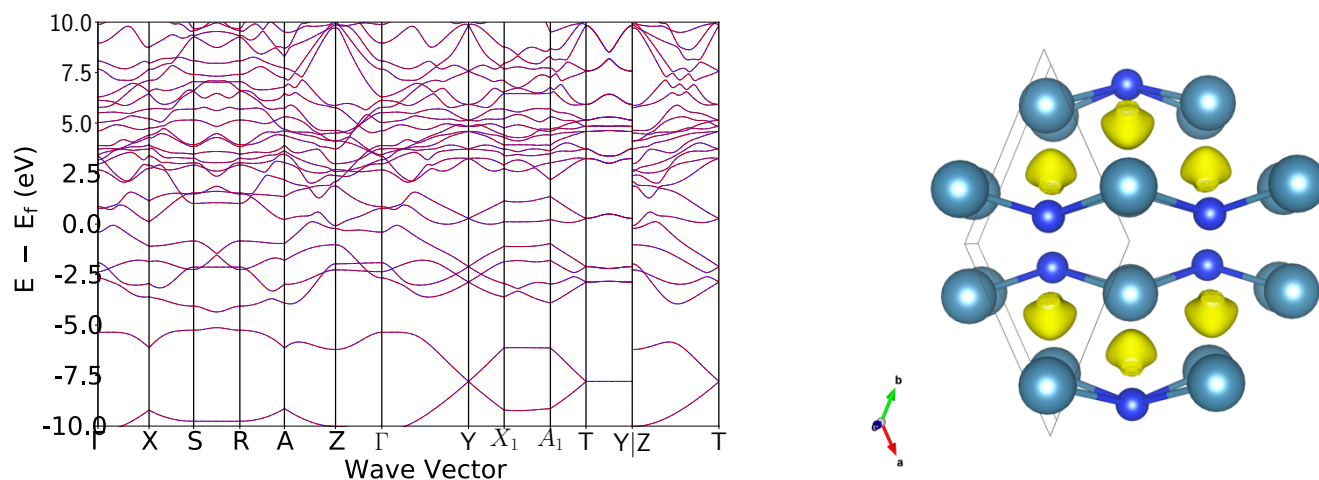


Figure 15: CaSi (mp-1563). Symmetry: orthorhombic; Cmc_m (number 63). Structure: CrB-type. Origin: ICSD;¹⁴ comments: high pressure phase, *ab initio* predicted structure. CaSi described as 'Zintl compound'. Electron localization function shows anion covalency 'proving Zintl concept'. ELF also shows 'lone pair regions' in structure. High pressure can induce bonding interactions between cations in similar structures. Anionic electron coordination environment: distorted octahedral with Ca and Si.

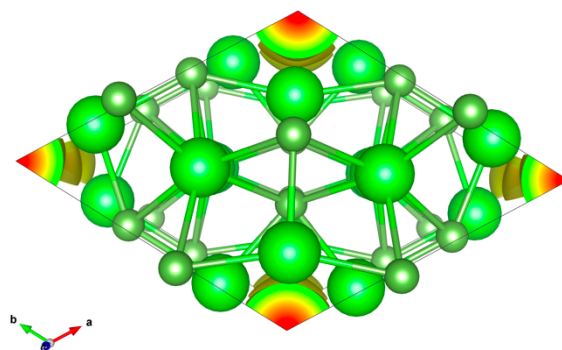
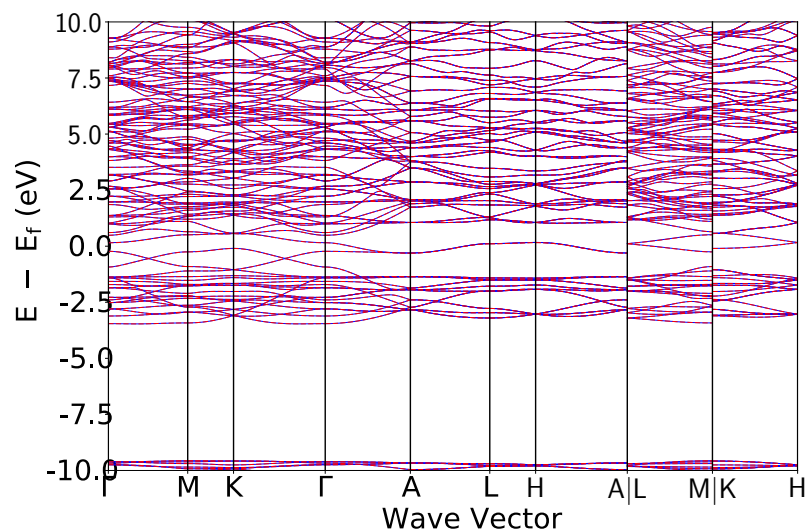


Figure 16: Sr_5As_3 (mp-15698). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD; ¹ comments: referred to as intermetallic. Anionic electron coordination environment: trigonal pyramidal with Sr.

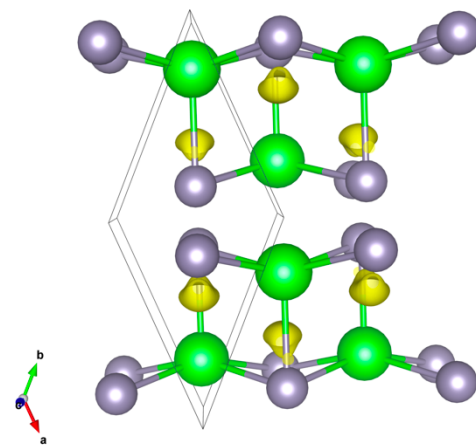
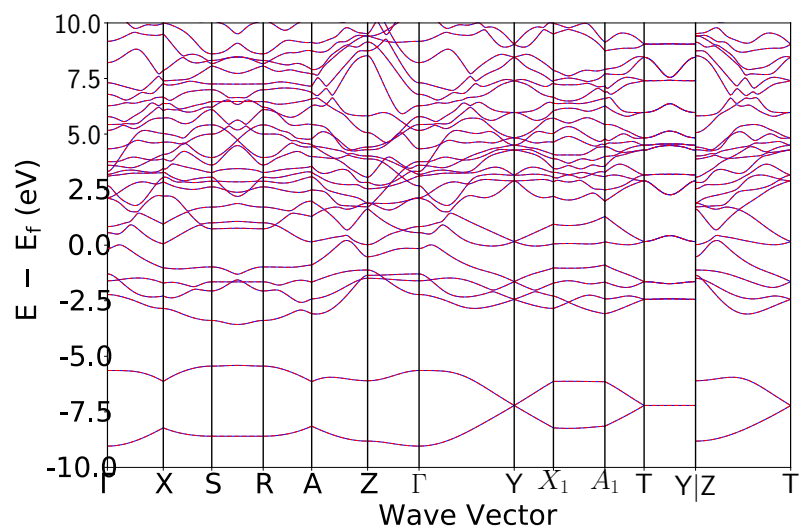


Figure 17: SrSn (mp-1698). Symmetry: orthorhombic; Cmcm (number 63). Structure: CrB-type. Origin: ICSD;¹⁵ comments: N/A. Anionic electron coordination environment: distorted octahedral with Sr and Sn.

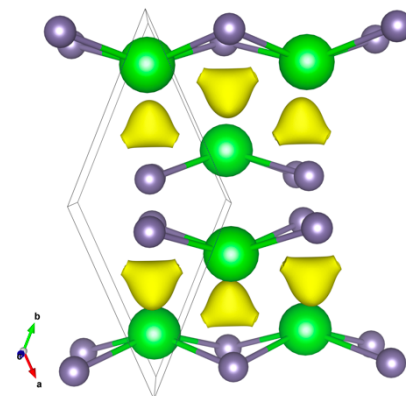
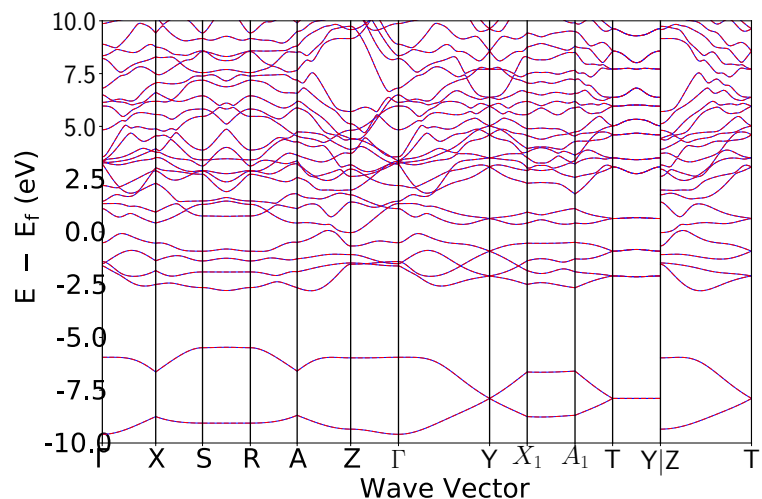


Figure 18: BaGe (mp-1730). Symmetry: orthorhombic; Cmcm (number 63). Structure: CrB-type. Origin: ICSD;¹⁶ comments: described as Zintl: “general valence equation suggests the presence of anion-anion chains”, reacts violently with moisture. Anionic electron coordination environment: distorted octahedral with Ba and Ge.

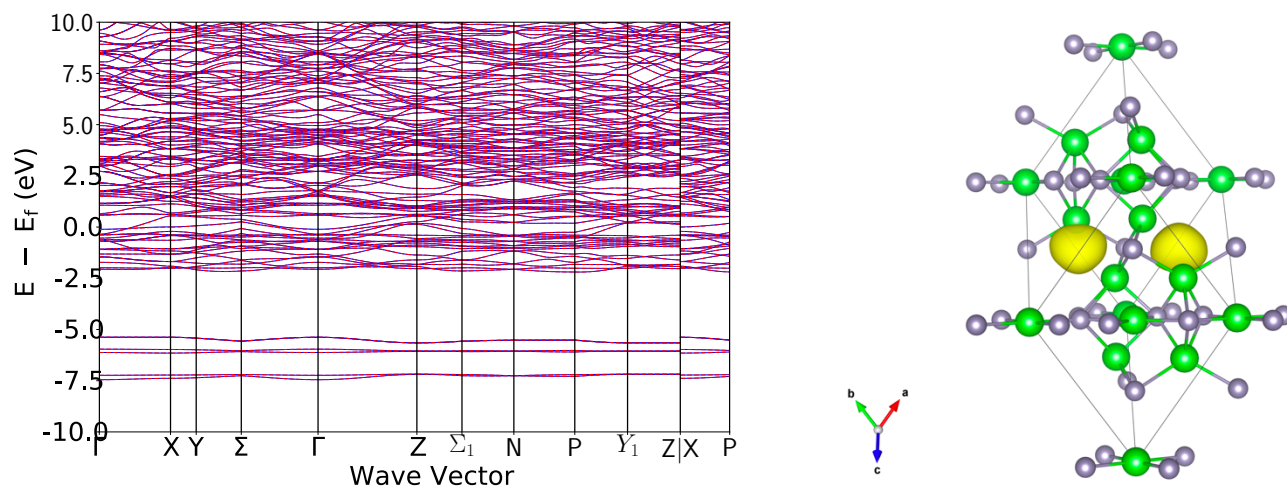


Figure 19: Ba₅Sn₃ (mp-17325). Symmetry: tetragonal; 14/mcm (number 140). Structure: Cr₅B₃-type. Origin: ICSD;¹⁷ comments: referred to as intermetallic. Anionic electron coordination environment: tetrahedral with Ba.

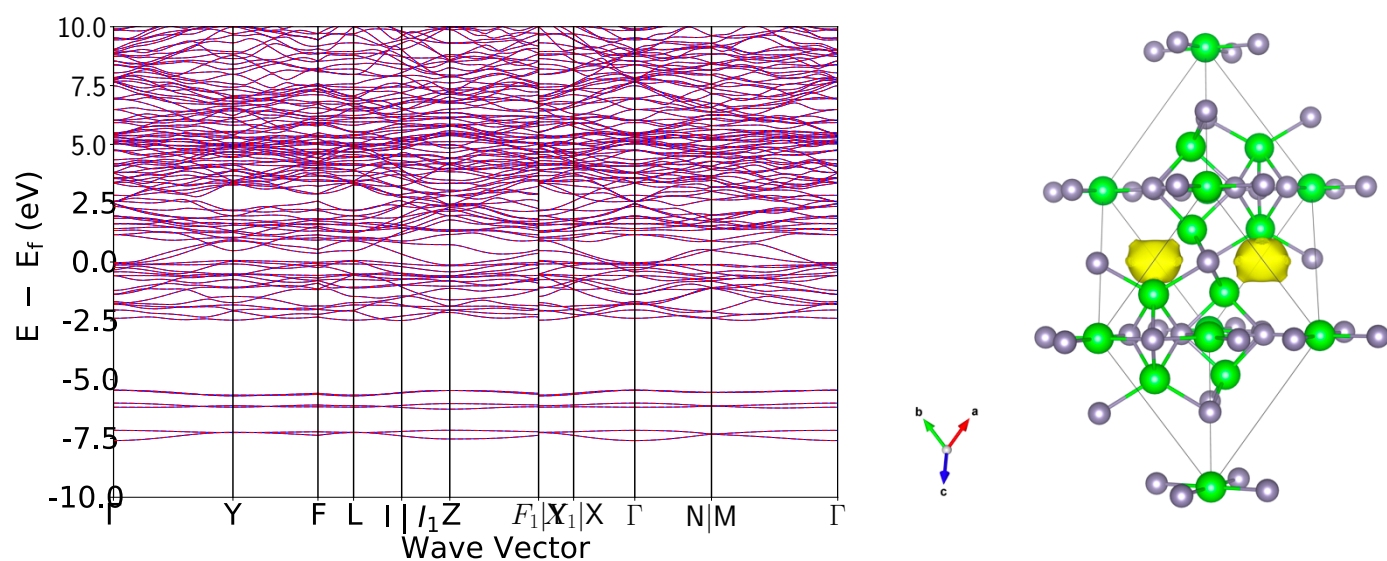


Figure 20: Sr₅Sn₃ (mp-17720). Symmetry: tetragonal; 14/mcm (number 140). Structure: Cr₅B₃-type. Origin: ICSD;¹⁷ comments: referred to as intermetallic. Anionic electron coordination environment: tetrahedral with Sr.

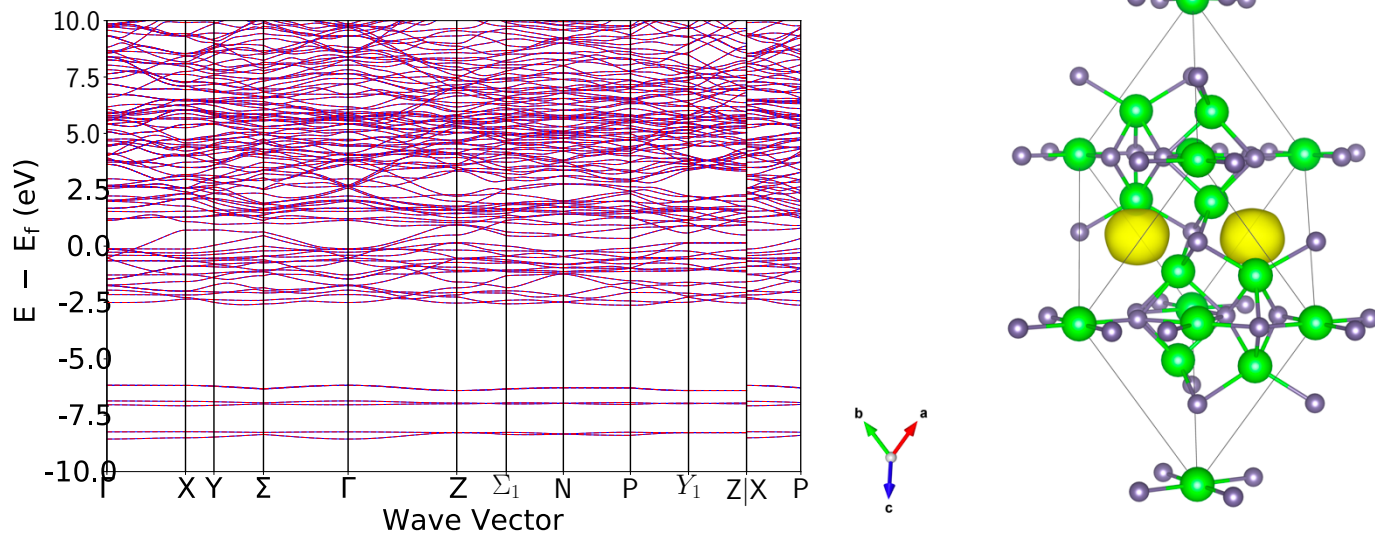


Figure 21: Sr₅Ge₃ (mp-17757). Symmetry: tetragonal; 14/mcm (number 140). Structure: Cr₅B₃-type. Origin: ICSD;¹⁸ comments: referred to as Zintl compound. Anionic electron coordination environment: tetrahedral with Sr.

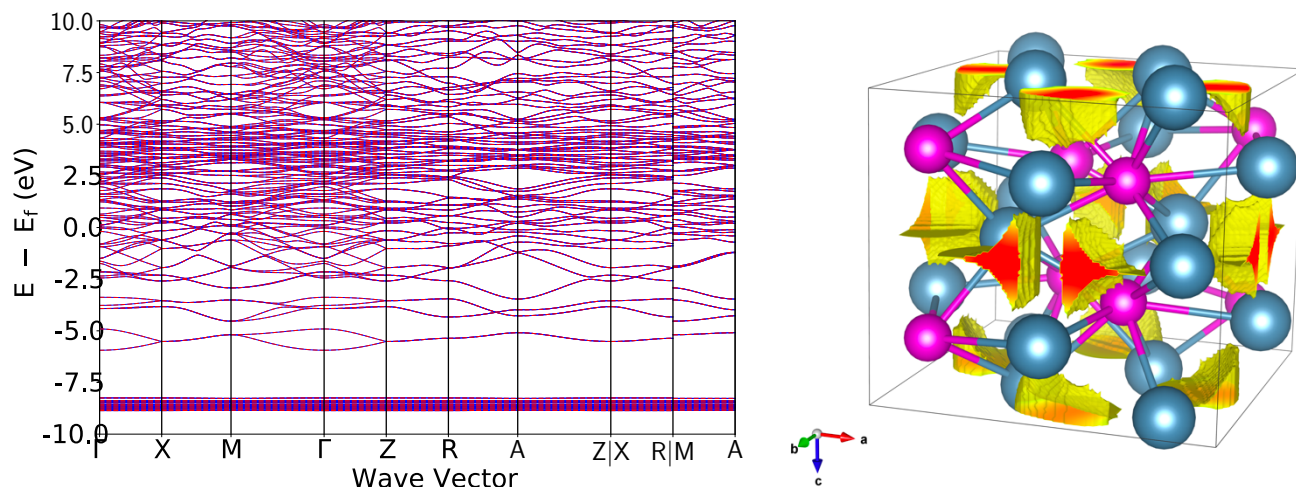


Figure 22: Ca_3Cd_2 (mp-18167). Symmetry: tetragonal; $P4_2/mnm$ (number 136). Structure: Gd_3Al_2 -type. Origin: ICSD;¹⁹ comments: referred to as intermetallic. Anionic electron coordination environment: tetrahedral with Ca.

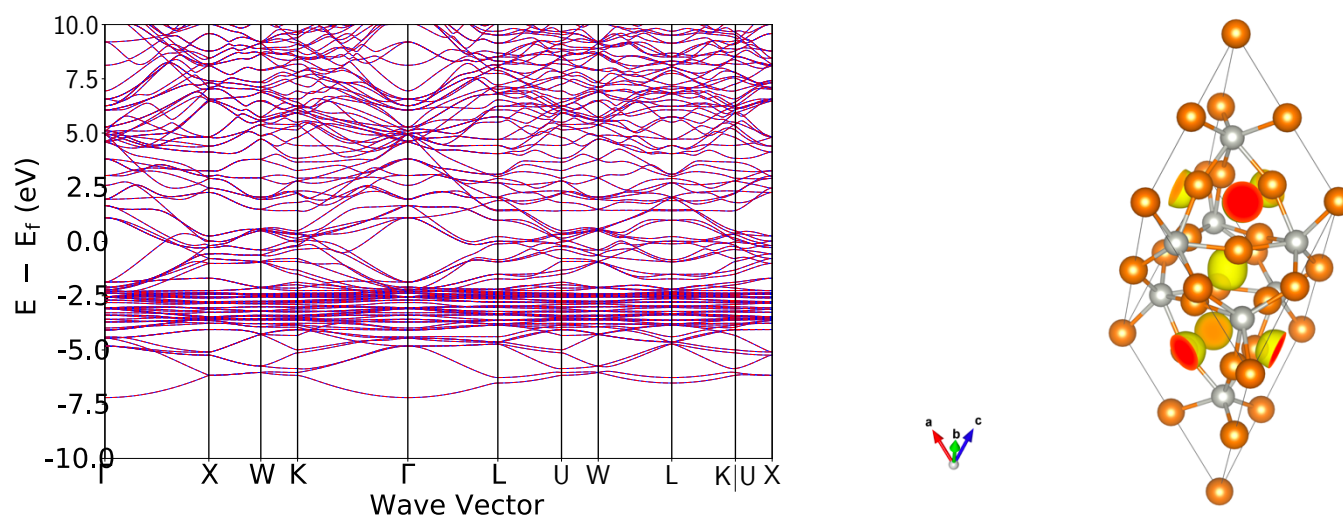


Figure 23: Mg_2Pd (mp-18316). Symmetry: cubic; $Fd\bar{3}m$ (number 227). Structure: NiTi_2 -type. Origin: ICSD;²⁰ comments: N/A. Anionic electron coordination environment: octahedral with Mg.

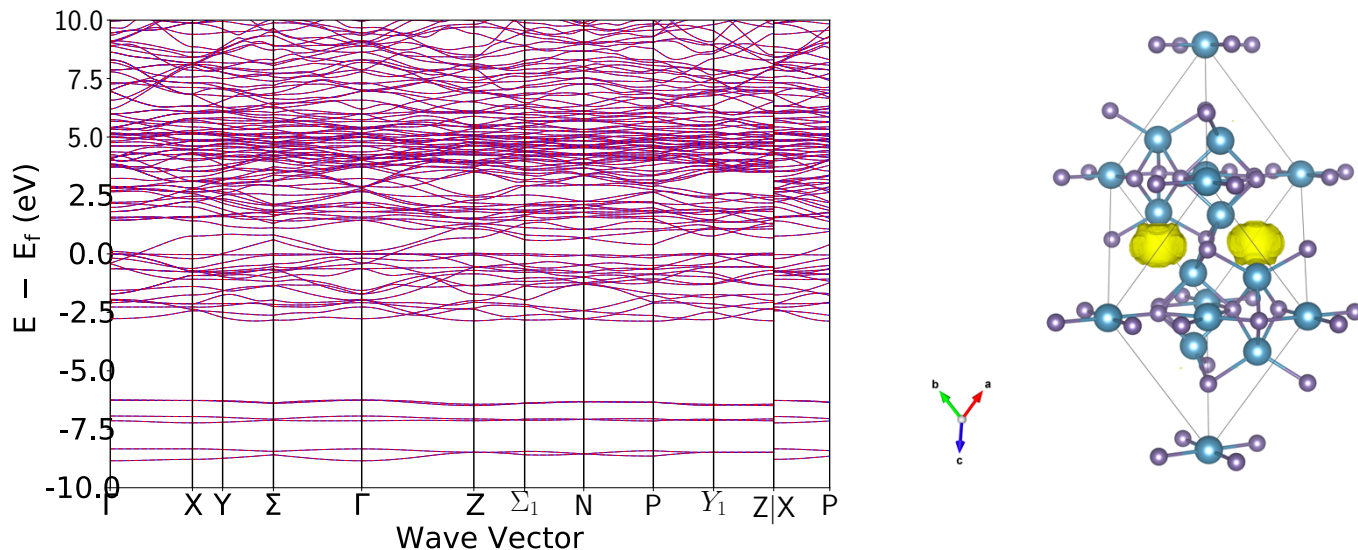


Figure 24: Ca_5Ge_3 (mp-1884). Symmetry: tetragonal; $I4/mcm$ (number 140). Structure: Cr_5B_3 -type. Origin: ICSD;²¹ comments: referred to as Zintl phase. Suggest unresolved hydrogen might be included in structure. Anionic electron coordination environment: tetrahedral with Ca.

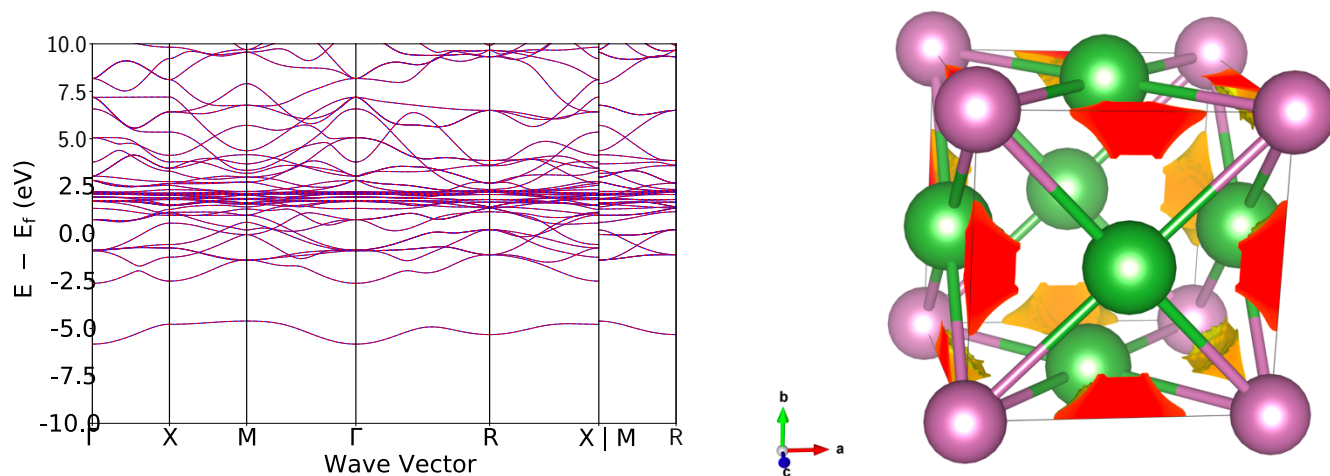


Figure 25: La_3In (mp-20909). Symmetry: cubic; $\text{Pm}\text{-}3\text{m}$ (number 221). Structure: Cu_3Au -type. Origin: ICSD;²² comments: superconductor at low temperature. Anionic electron coordination environment: octahedral with La and In.

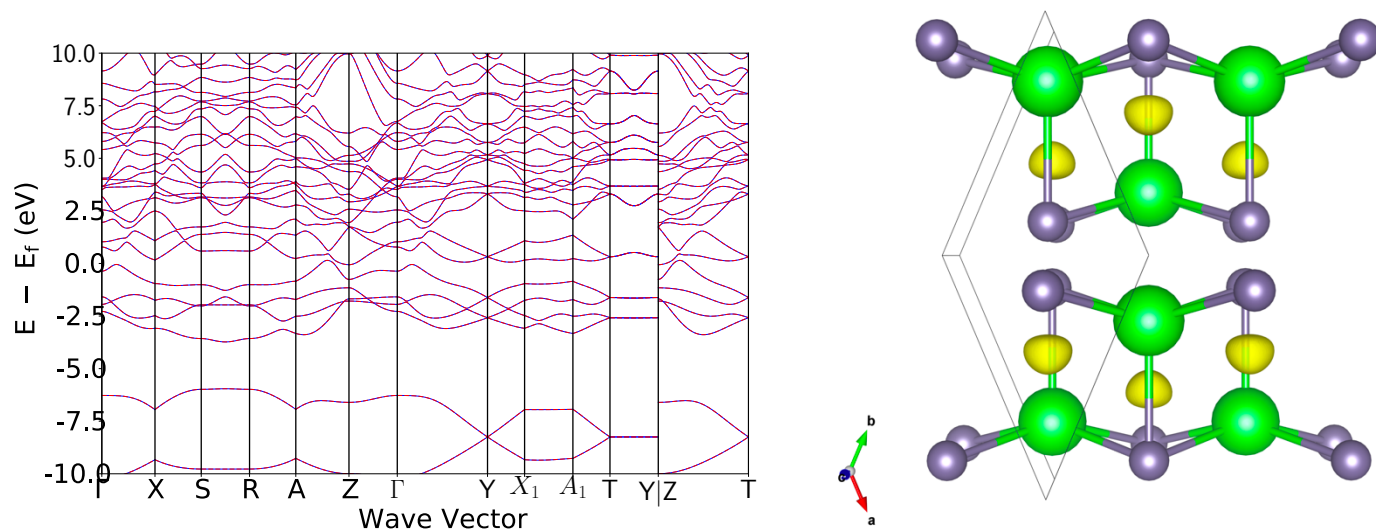


Figure 26: SrGe (mp-2147). Symmetry: orthorhombic; Cmcm (number 63). Structure: CrB -type. Origin: ICSD;¹⁶ comments: referred to as intermetallic. Anionic electron coordination environment: distorted octahedral with Sr and Ge.

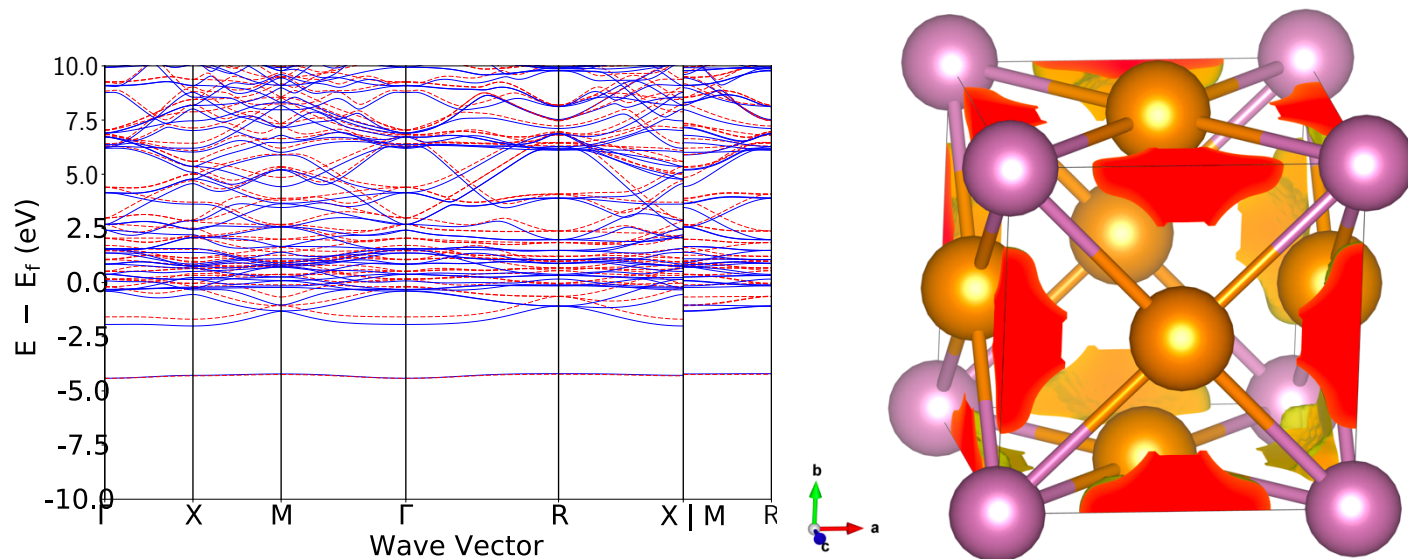


Figure 27: Nd_3In (mp-21483). Symmetry: cubic; $\text{Pm}\text{-}3\text{m}$ (number 221). Structure: Cu_3Au -type. Origin: ICSD;²³ comments: band splitting indicative of magnetism. Anionic electron coordination environment: octahedral with Nd and In.

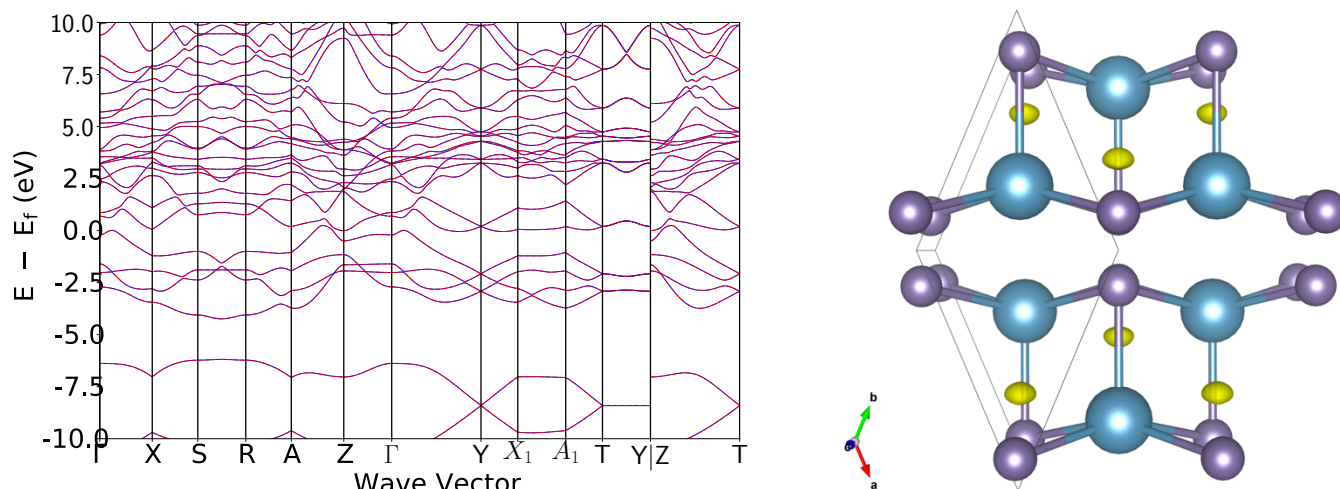


Figure 28: CaGe (mp-2360). Symmetry: orthorhombic; Cmc_m (number 63). Structure: CrB-type. Origin: ICSD;²⁴ comments: N/A. Anionic electron coordination environment: distorted octahedral with Ca and Ge.

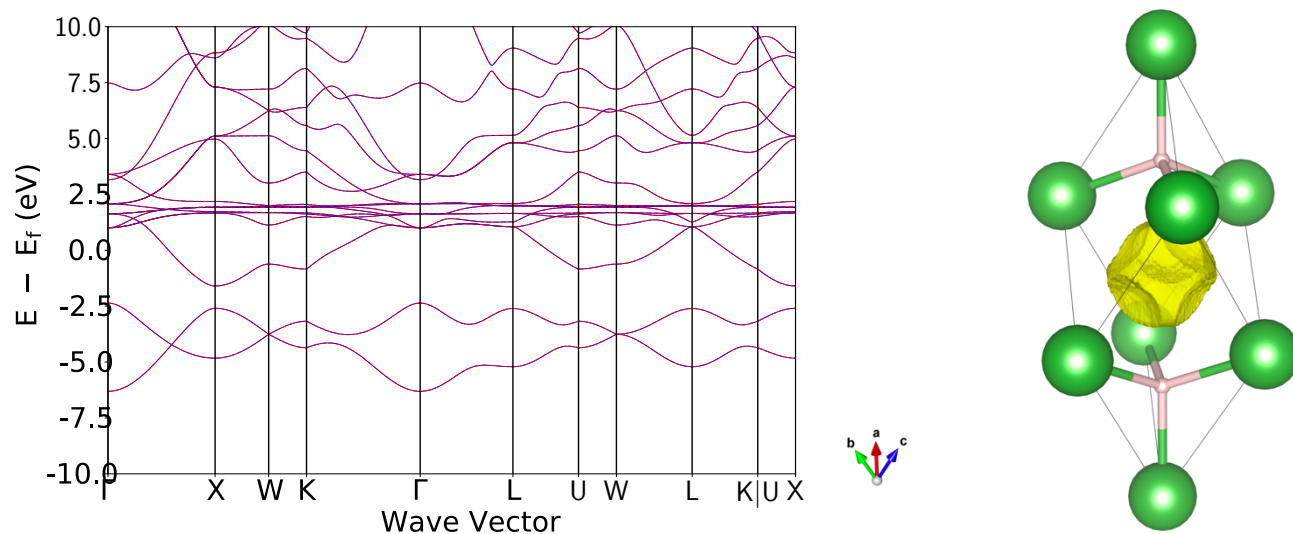


Figure 29: LaH₂ (mp-24153). Symmetry: cubic; Fm-3_m (number 225). Structure: CaF₂-type. Origin: ICSD;²⁵ comments: N/A. Anionic electron coordination environment: square-antiprismatic with H.

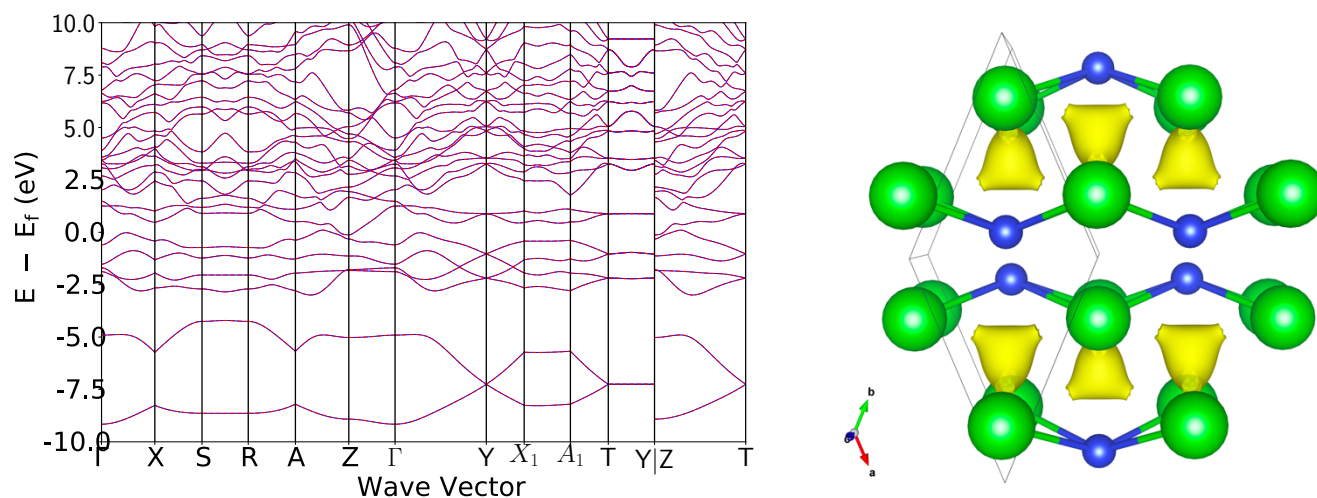


Figure 30: BaSi (mp-2499). Symmetry: orthorhombic; Cmc_m (number 63). Structure: CrB-type. Origin: ICSD;¹⁶ comments: referred to as intermetallic. Anionic electron coordination environment: tetrahedral with Ba.

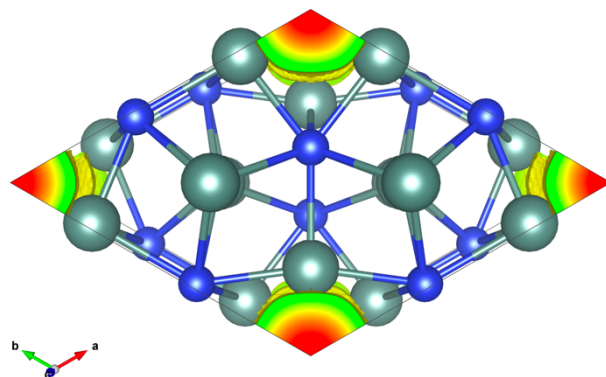
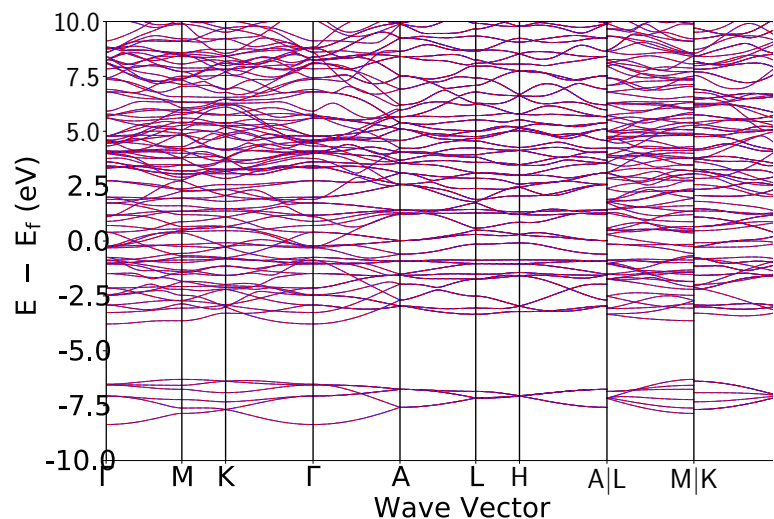


Figure 31: Y_5Si_3 (mp-2538). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD;²⁶ comments: Mn_5Si_3 -type compounds can be “stuffed” with variety of elements without change in lattice type. “Stuffed” compounds referred to as “Nowotny” phases. Y_5Si_3 successfully subject to boron intercalation. Anionic electron coordination environment: octahedral with Y.

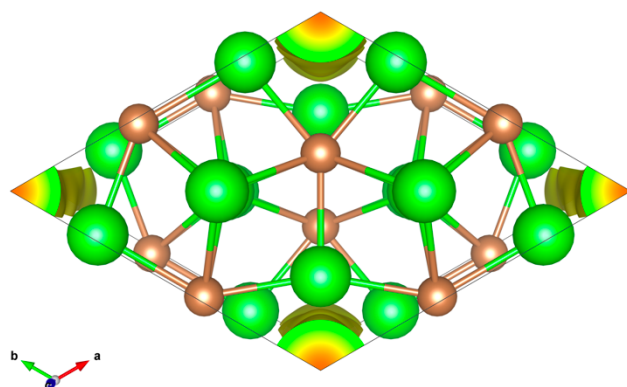
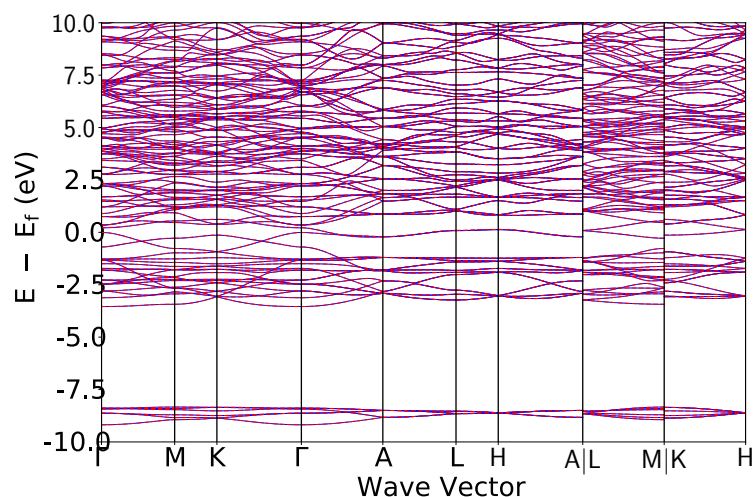


Figure 32: Sr_5Sb_3 (mp-2585). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD;²⁷ comments: referred to as Zintl. Anionic electron coordination environment: trigonal planar with Sr.

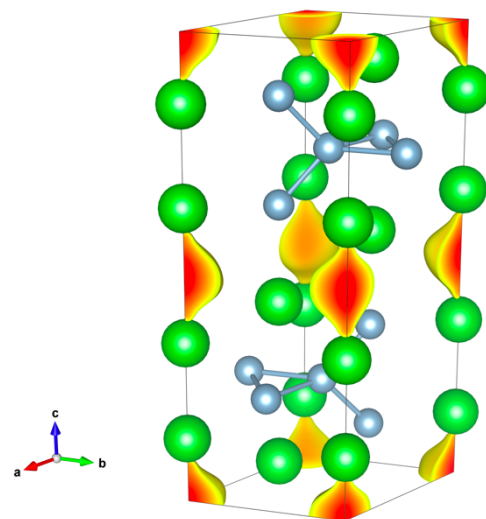
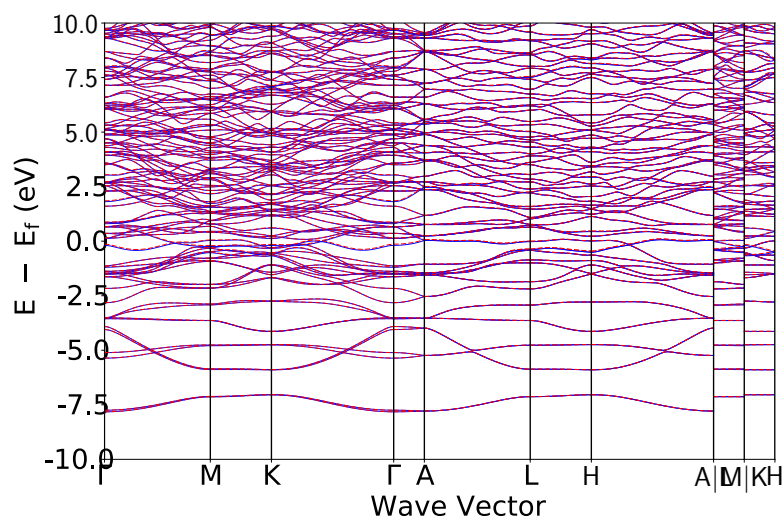


Figure 33: Ba_4Al_5 (mp-2631). Symmetry: hexagonal; $P6_3/mmc$ (number 194). Structure: Ba_4Al_5 -type. Origin: ICSD;²⁸ comments: referred to as Zintl compound. “Al atoms the polyanion should bear a charge of minus 7 which means that the number of counter cations is... too large in Ba_4Al_5 ”. “Possible hydrogen impurities can be ruled out”. Anionic electron coordination environment: linear with Ba.

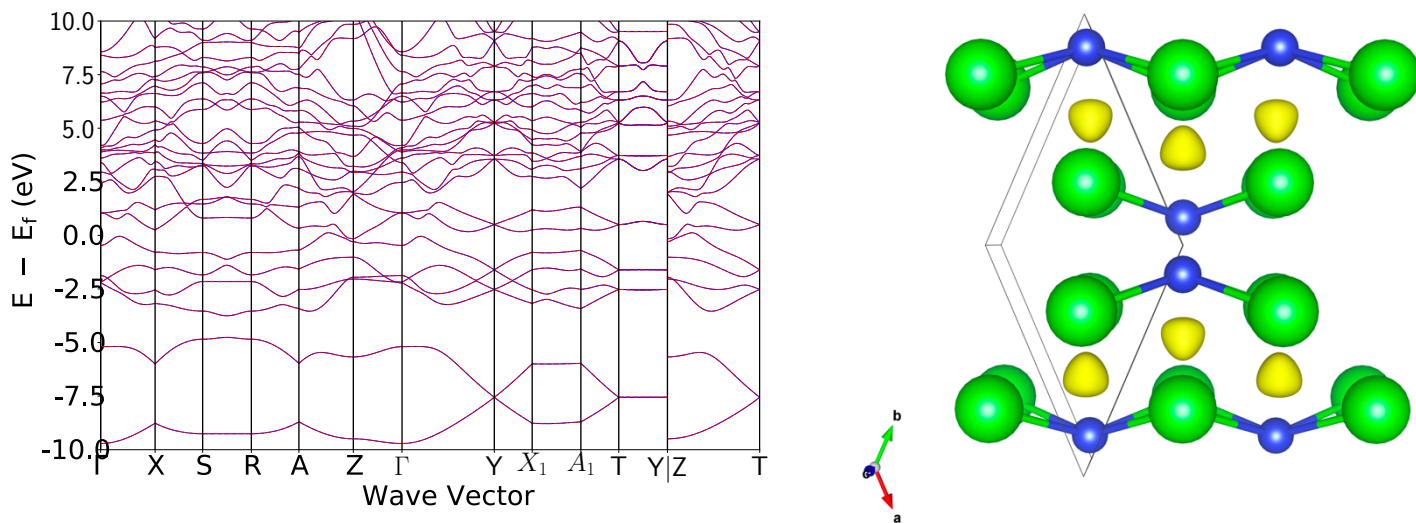


Figure 34: SrSi (mp-2661). Symmetry: orthorhombic; Cmc_m (number 63). Structure: CrB-type. Origin: ICSD;⁹ *ab initio* predicted structure. Anionic electron coordination environment: distorted octahedral with Sr and Si.

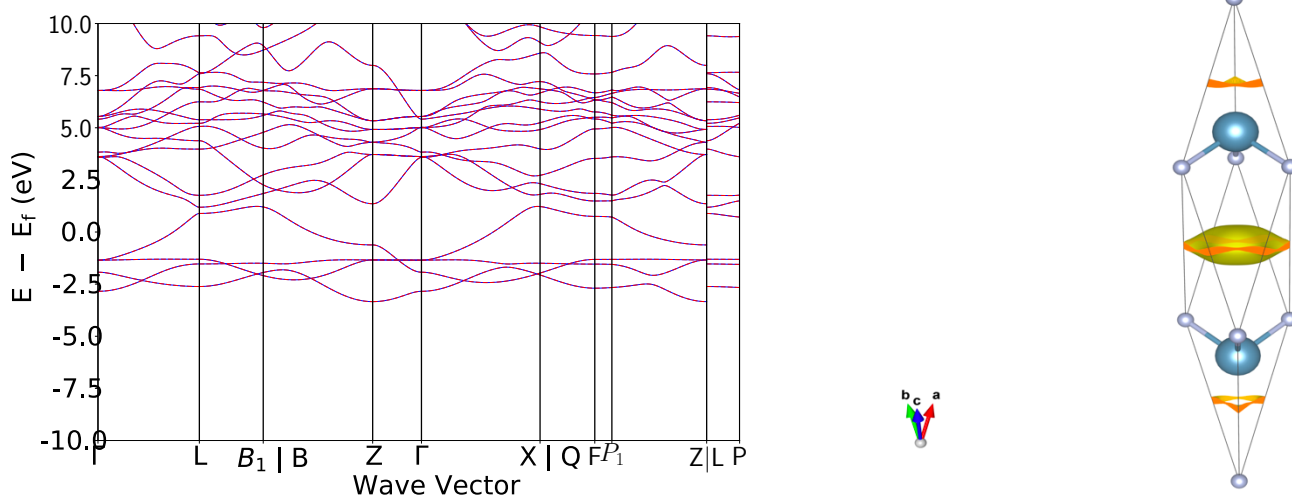


Figure 35: Ca₂N (mp-2686). Symmetry: trigonal; R-3_m (number 166). Structure: anti-CdCl₂-type. Origin: ICSD;²⁹ comments: describes 'metallic inter-layer bonding' of 'nearly free remaining electrons'. Refers to as 'void metal'. 'the metallicly bonded regions are more compressible than the ionically bonded ones... compressibility along the *c*-axis was found to be about twice as high compared to that along the *a*-axis'. Anionic electron coordination environment: octahedral with Ca.

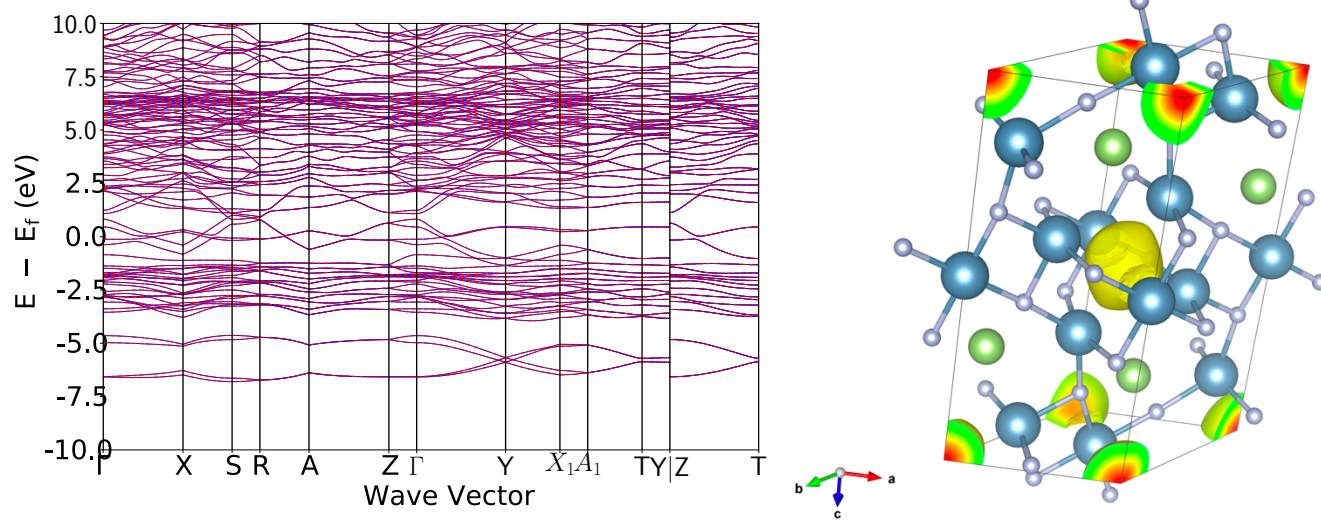


Figure 36: Ca₅(GaN₂)₂ (mp-28489). Symmetry: orthorhombic; Cmca (number 64). Structure: Ca₅(GaN₂)₂-type. Origin: ICSD;³⁰ comments: referred to as Zintl phase. Anionic electron coordination environment: octahedral with Ca.

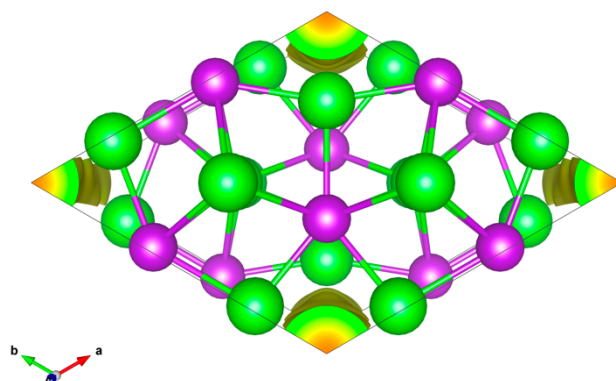
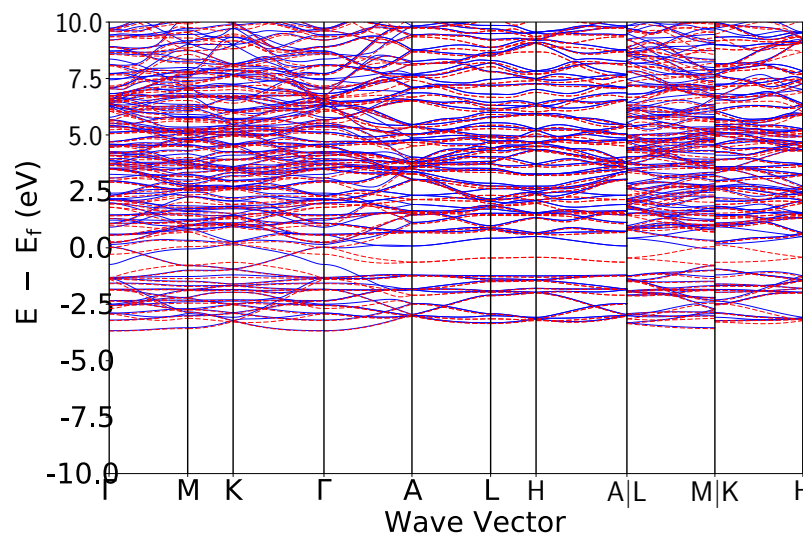


Figure 37: Sr_5Bi_3 (mp-29620). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD;³¹ comments: band splitting indicative of magnetism. Anionic electron coordination environment: trigonal planar with Sr.

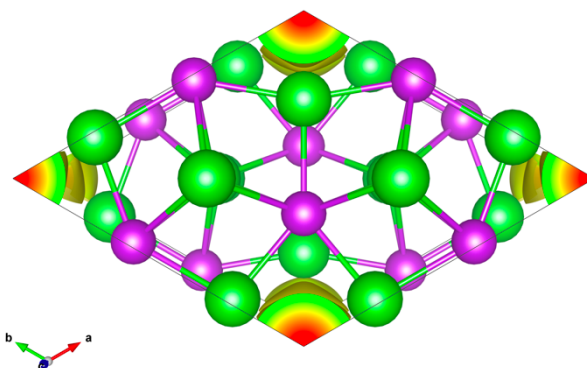
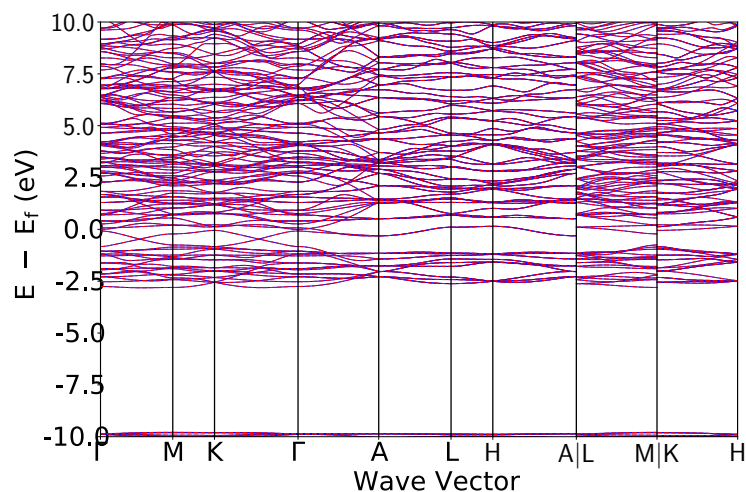


Figure 38: Ba_5Bi_3 (mp-29621). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD;³¹ comments: N/A. Anionic electron coordination environment: octahedral with Ba.

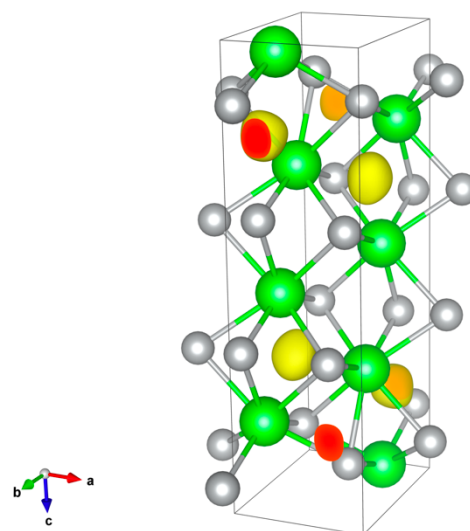
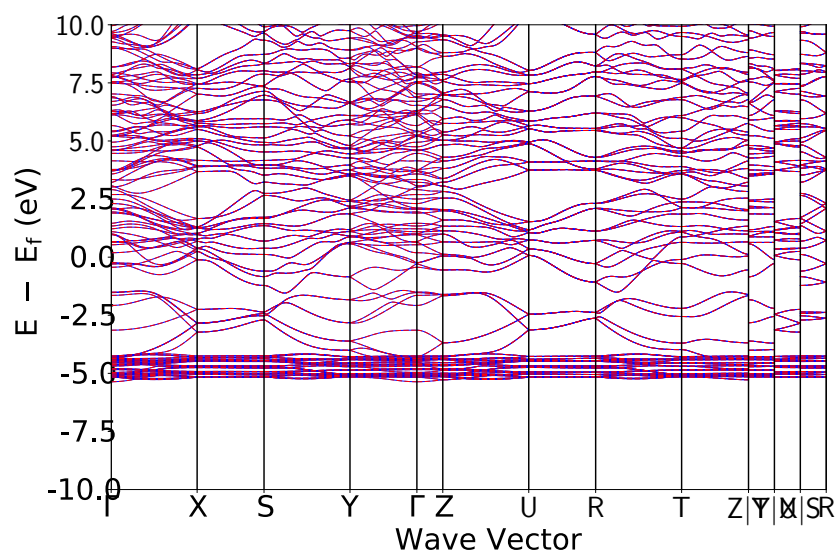


Figure 39: SrAg (mp-30355). Symmetry: Orthorhombic; $Pnma$ (number 62). Structure: SrAg -type. Origin: ICSD;⁴ comments: N/A. Anionic electron coordination environment: distorted octahedral with Sr and Ag.

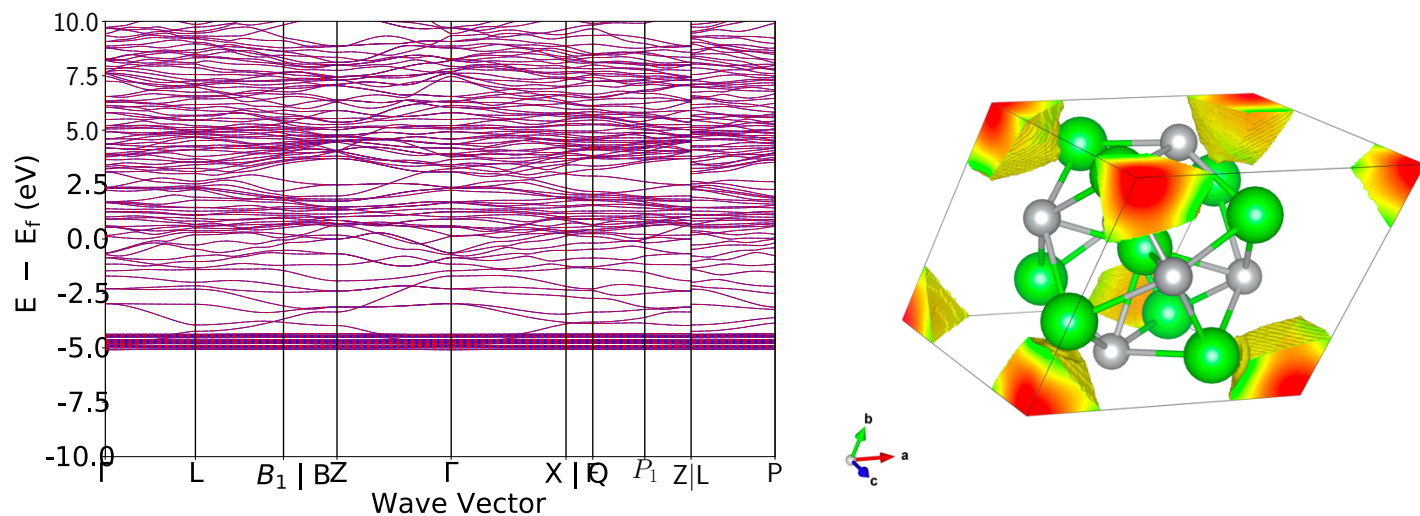


Figure 40: Sr_3Ag_2 (mp-30357). Symmetry: trigonal; R-3 (number 148). Structure: Er_3Ni_2 -type. Origin: ICSD;³² comments: N/A. Anionic electron coordination environment: octahedral with Sr.

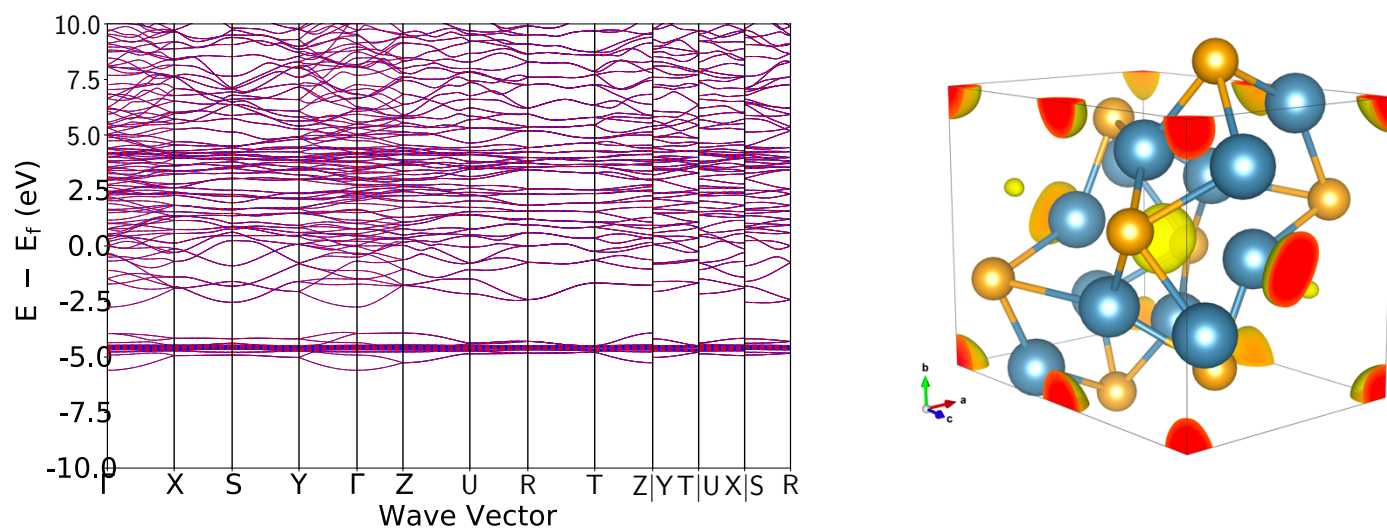


Figure 41: Ca_3Au (mp-30366). Symmetry: Orthorhombic; Pnma (number 62). Structure: Ca_3Au -type. Origin: ICSD;³³ comments: N/A. Anionic electron coordination environment: octahedral with Ca.

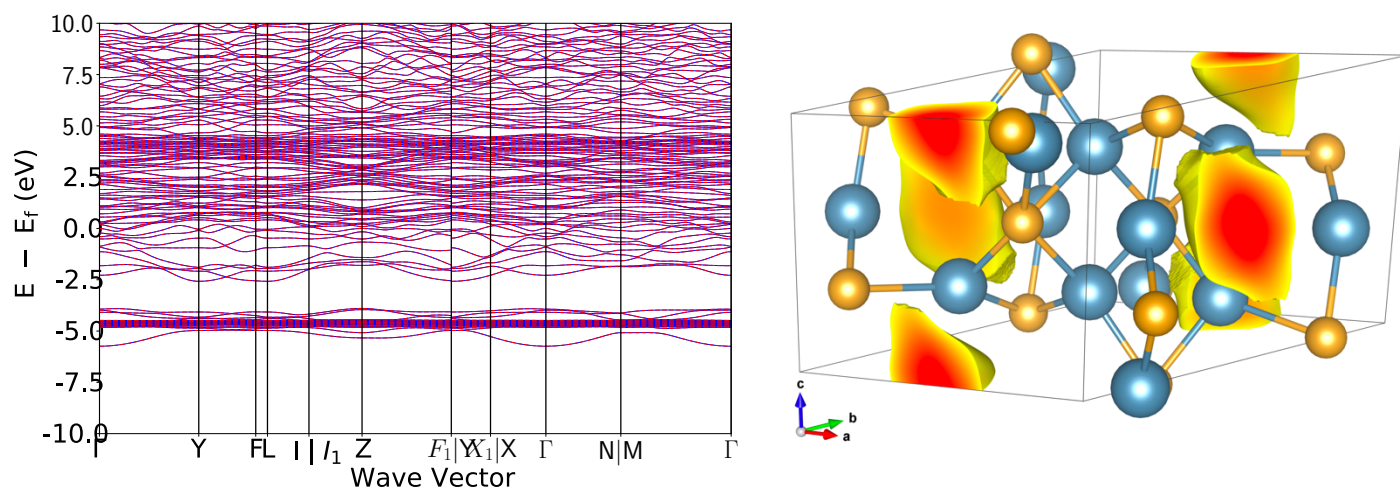


Figure 42: Ca_5Au_2 (mp-30367). Symmetry: Monoclinic; C2/c (number 15). Structure: Ca_5Au_2 -type. Origin: ICSD;³³ comments: N/A. Anionic electron coordination environment: octahedral with Ca.

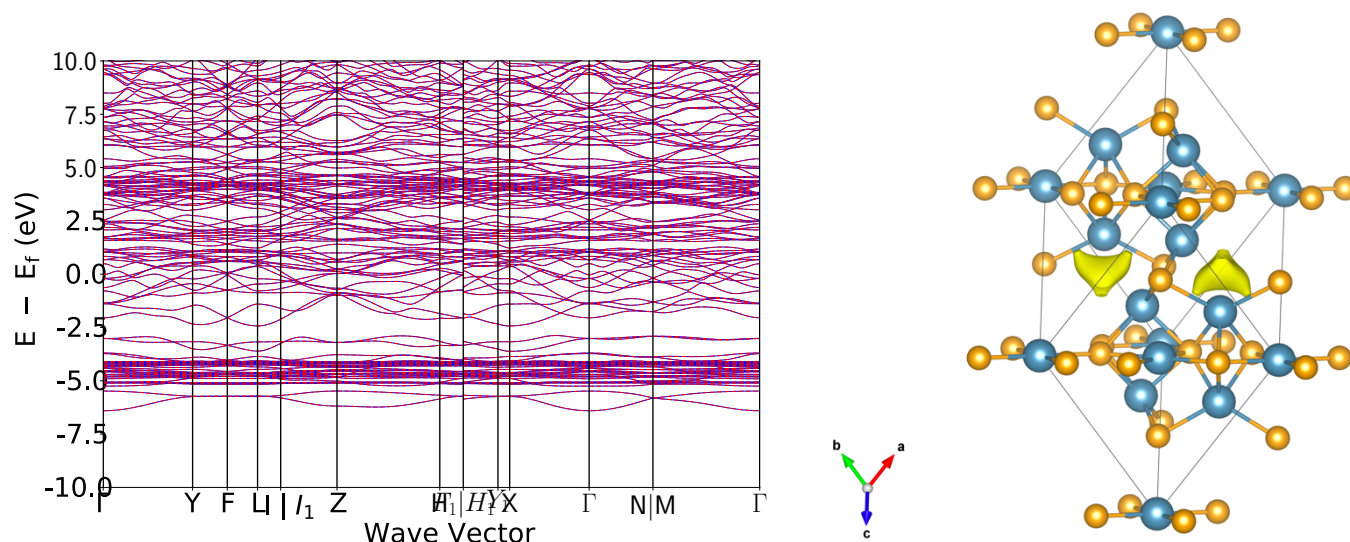


Figure 43: Ca_5Au_3 (mp-30368). Symmetry: tetragonal; $I4/mcm$ (number 140). Structure: Cr_5B_3 -type. Origin: ICSD;³² comments: N/A. Anionic electron coordination environment: tetrahedral with Ca.

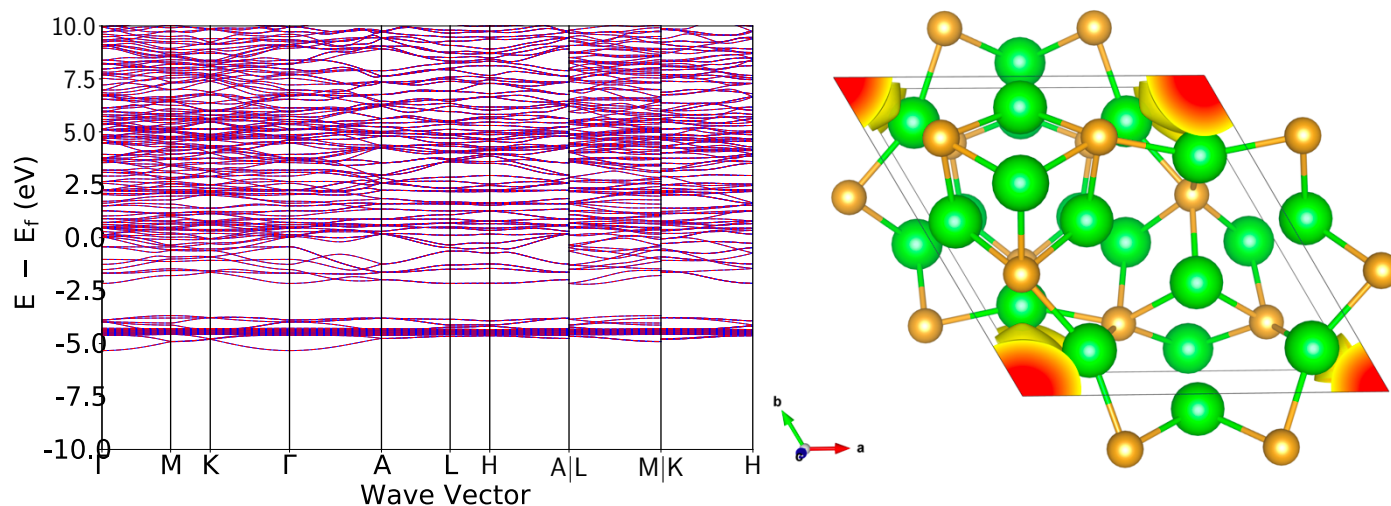


Figure 44: Sr_7Au_3 (mp-30422). Symmetry: hexagonal; $P6_3/mc$ (number 186). Structure: Sr_7Au_3 -type. Origin: ICSD;³² comments: N/A. Anionic electron coordination environment: octahedral with Sr.

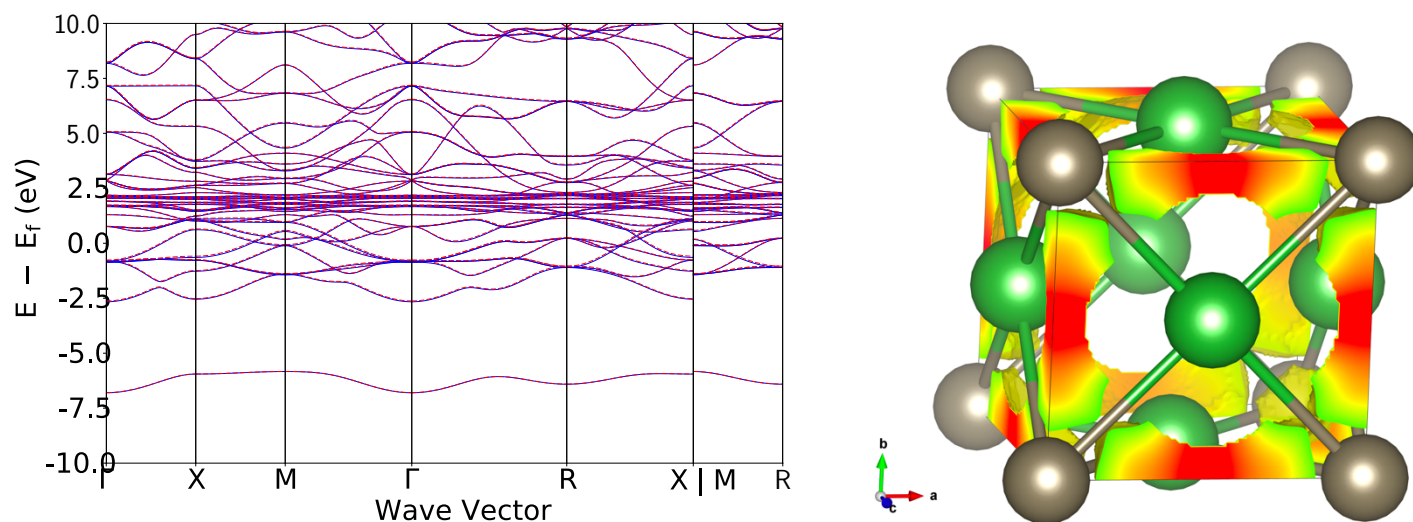


Figure 45: La_3Tl (mp-371). Symmetry: cubic; $Pm\bar{3}m$ (number 221). Structure: Cu_3Au -type. Origin: ICSD;²³ comments: N/A. Anionic electron coordination environment: octahedral with La and Tl.

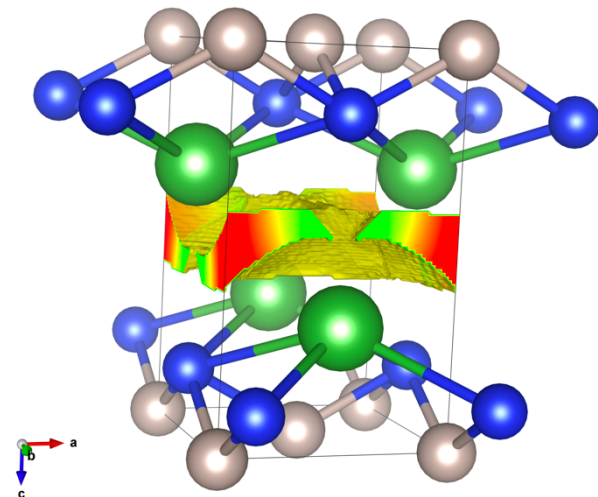
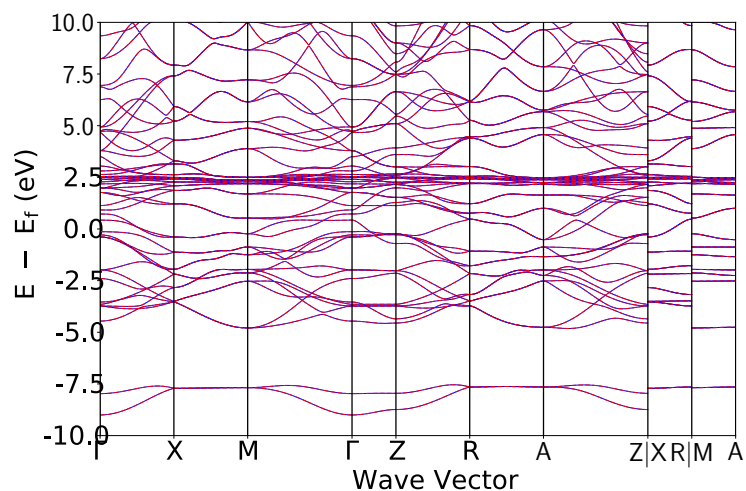


Figure 46: LaSiRu (mp-4579). Symmetry: tetragonal; $P4/nmm$ (number 129). Structure: LaSiRu-type. Origin: ICSD;³⁴ comments: N/A. Anionic electron coordination environment: tetrahedral with La.

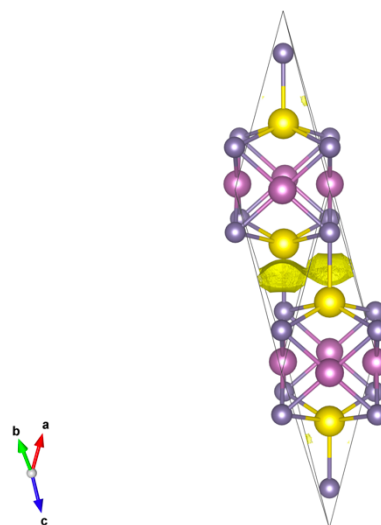
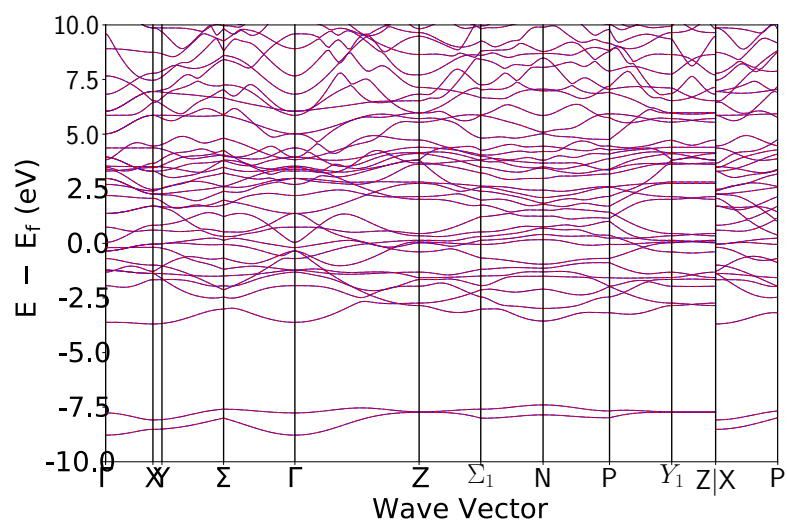


Figure 47: PrScGe (mp-4738). Symmetry: tetragonal; $I4/mmm$ (number 139). Structure: CeScSi-type. Origin: ICSD;³⁵ comments: “PrScGe demonstrates antiferromagnetic transition below $T_N = 140$ K, but below 83 K trends to ferromagnetic-type ordering”. Anionic electron coordination environment: tetrahedral with Pr.

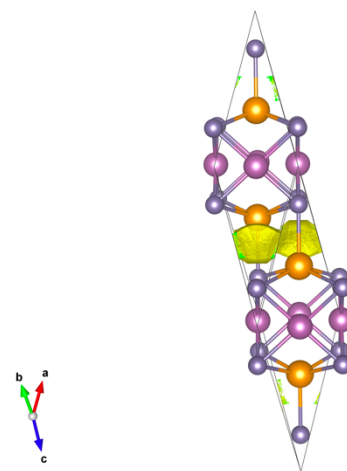
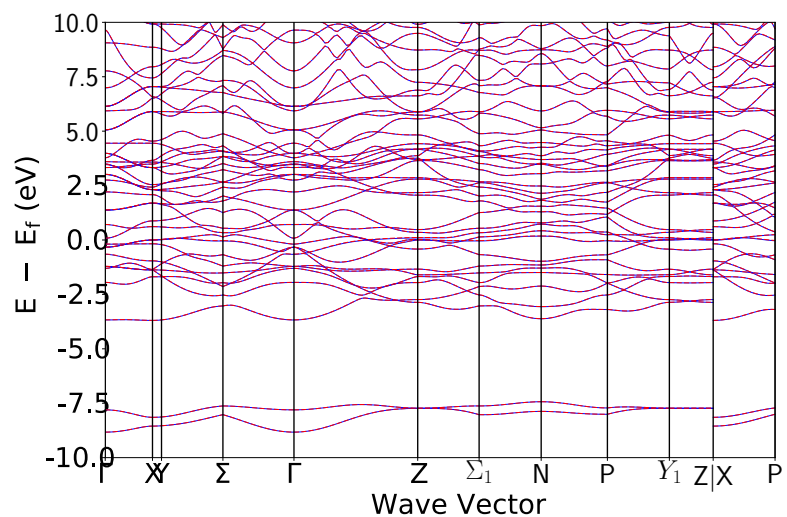


Figure 48: NdScGe (mp-4854). Symmetry: tetragonal; $I4/mmm$ (number 139). Structure: CeScSi-type. Origin: ICSD;³⁵ comments: N/A. Anionic electron coordination environment: tetrahedral with Nd.

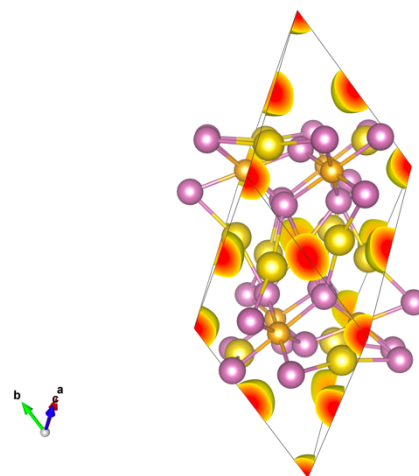
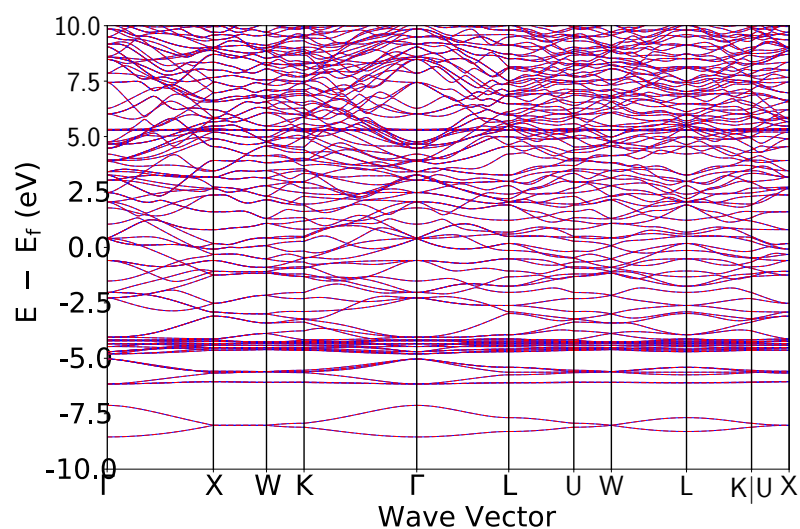


Figure 49: $\text{Na}_3\text{In}_2\text{Au}$ (mp-542680). Symmetry: cubic; $Fd\bar{3}m$ (number 227). Structure: NiTi_2 -type. Origin: ICSD;³⁶ comments: compared to 'well-known Zintl-phase'. Anionic electron coordination environment: octahedral with Na.

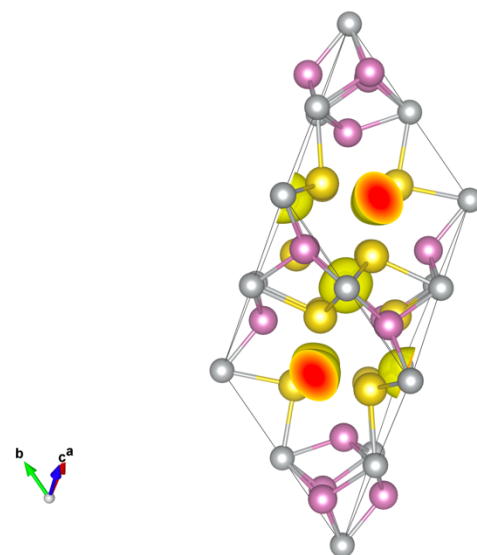
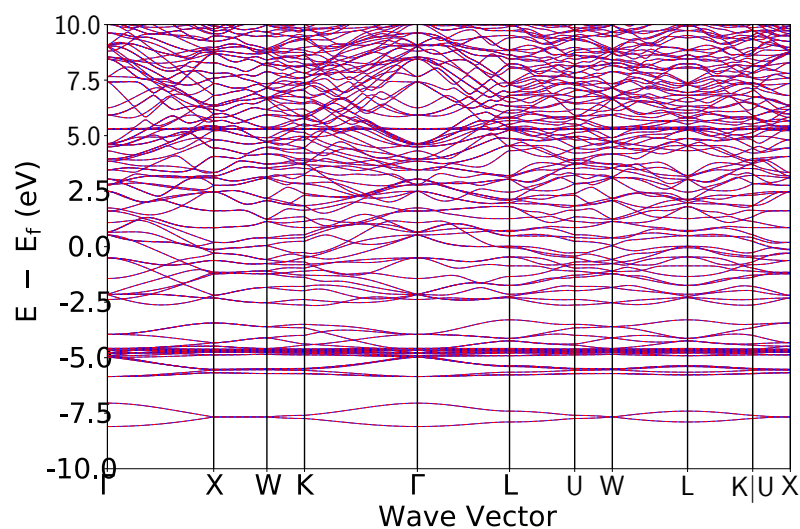


Figure 50: $\text{Na}_3\text{In}_2\text{Ag}$ (mp-542681). Symmetry: cubic; $Fd\bar{3}m$ (number 227). Structure: NiTi_2 -type. Origin: ICSD;³⁶ comments: compared to 'well-known Zintl-phase'. Anionic electron coordination environment: octahedral with Na.

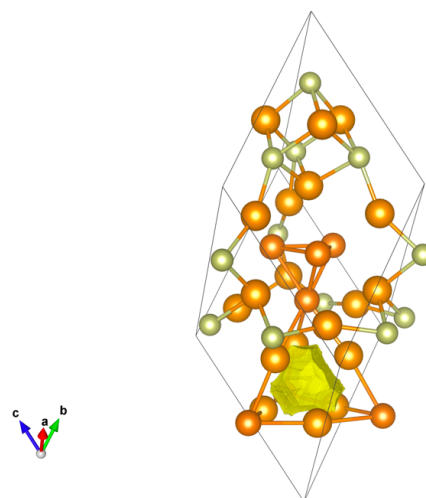
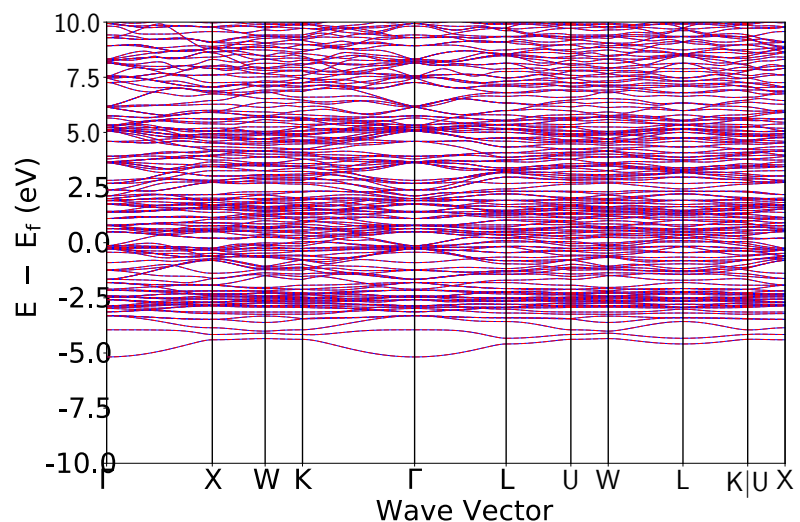


Figure 51: Nd_4MgIr (mp-567342). Symmetry: cubic; $F\bar{4}3m$ (number 216). Structure: NiTi_2 -type. Origin: ICSD;³⁷ comments: referred to as intermetallic. Anionic electron coordination environment: octahedral with Nd.

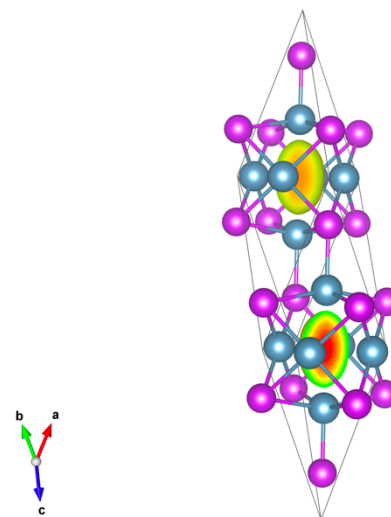
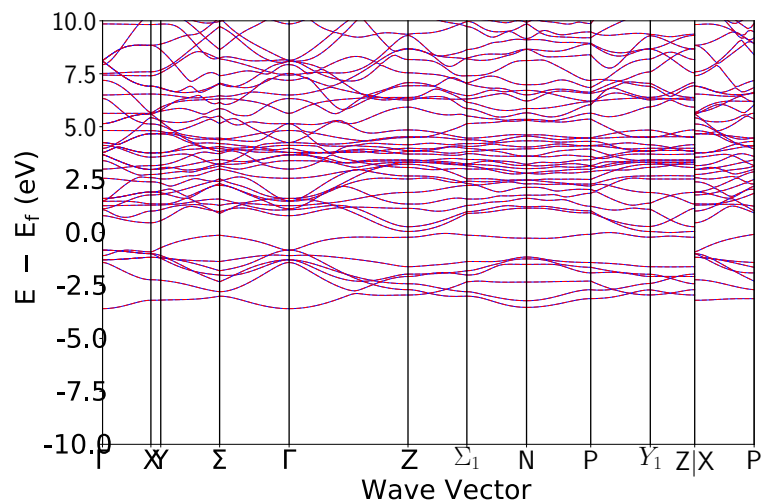


Figure 52: Ca_2Bi (mp-569535). Symmetry: tetragonal; $I4/mmm$ (number 139). Structure: CeScSi-type. Origin: ICSD;³⁸ comments: N/A. Anionic electron coordination environment: octahedral with Ca.

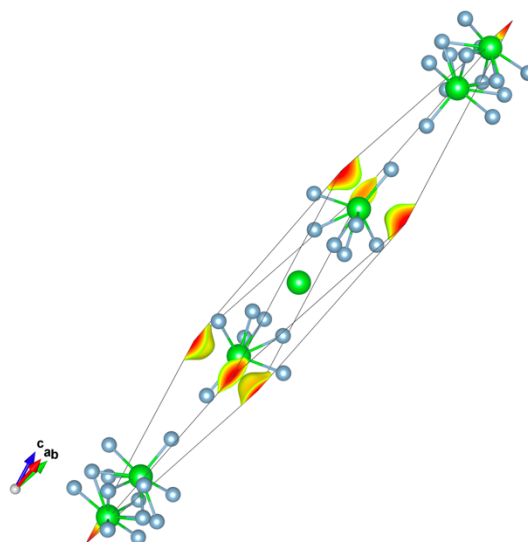
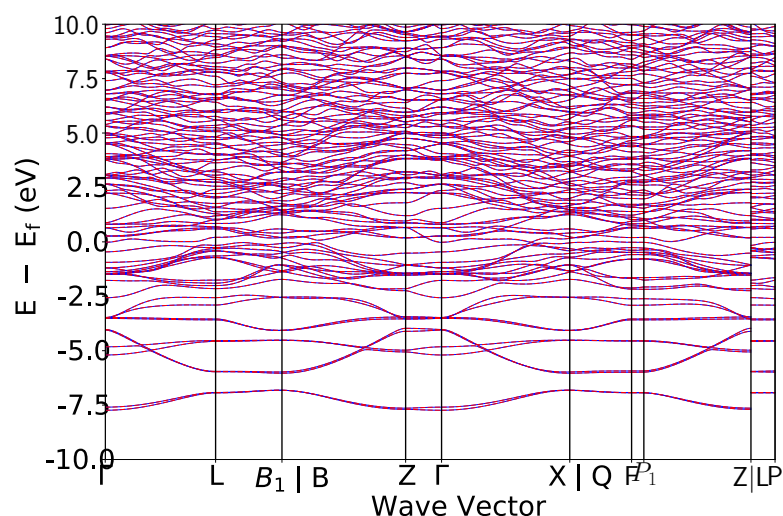


Figure 53: $\text{Ba}_7\text{Al}_{10}$ (mp-570400). Symmetry: trigonal; $R\bar{3}m$ (number 166). Structure: $\text{Ba}_7\text{Al}_{10}$ -type. Origin: ICSD;²⁸ comments: referred to as Zintl compound. Anionic electron coordination environment: linear with Ba.

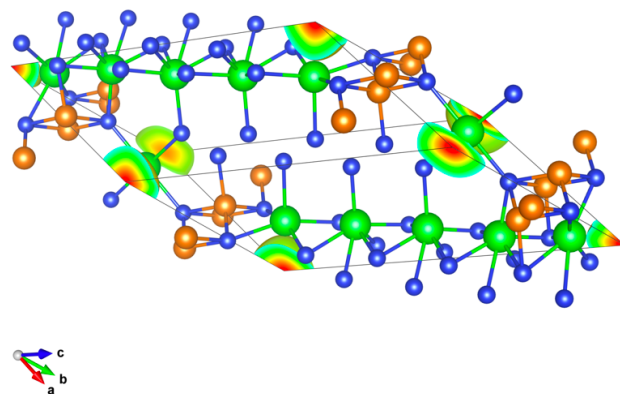
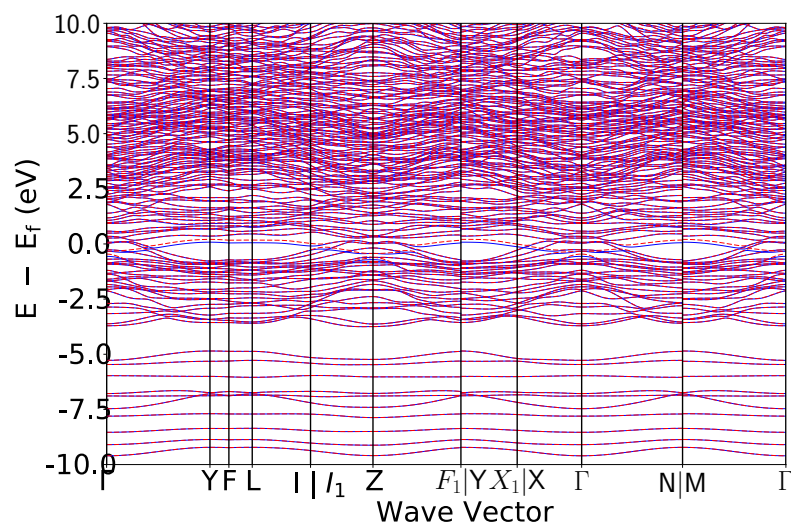


Figure 54: $\text{Sr}_{11}(\text{MgSi}_5)_2$ (mp-573908). Symmetry: monoclinic; $C2/m$ (number 12). Structure: $\text{Ba}_7\text{Al}_{10}$ -type. Origin: ICSD;³⁹ comments: band splitting indicative of magnetism. Anionic electron coordination environment: linear with Sr.

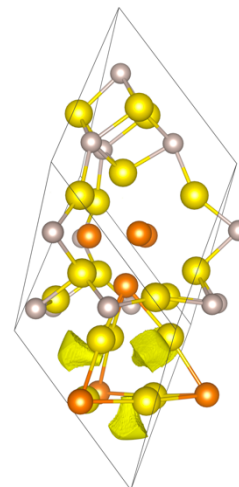
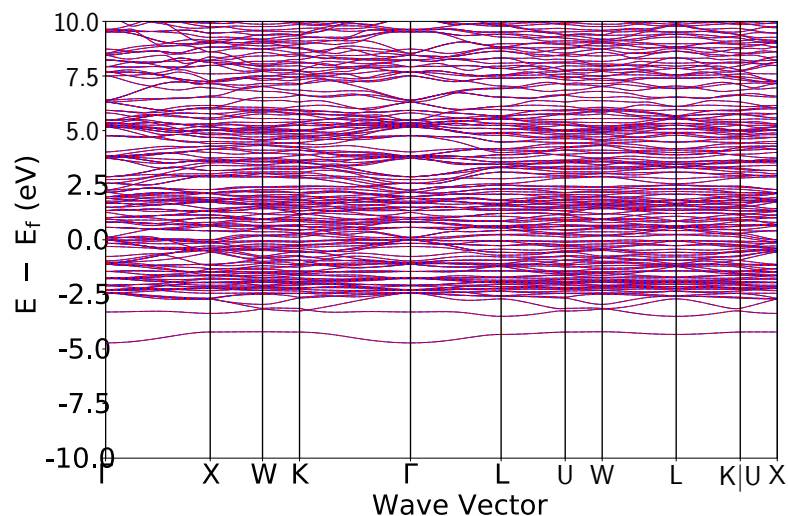


Figure 55: Pr_4MgRu (mp-605873). Symmetry: cubic; $F\bar{4}3m$ (number 216). Structure: NiTi_2 -type. Origin: ICSD;⁴⁰ comments: N/A. Anionic electron coordination environment: trigonal prismatic with Pr.

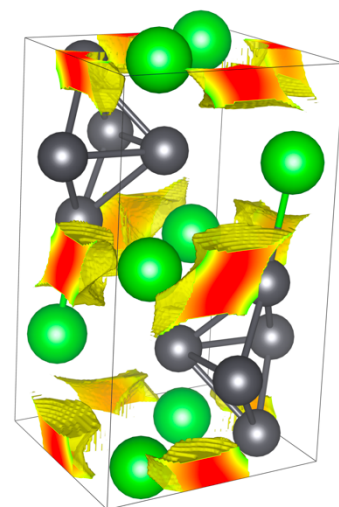
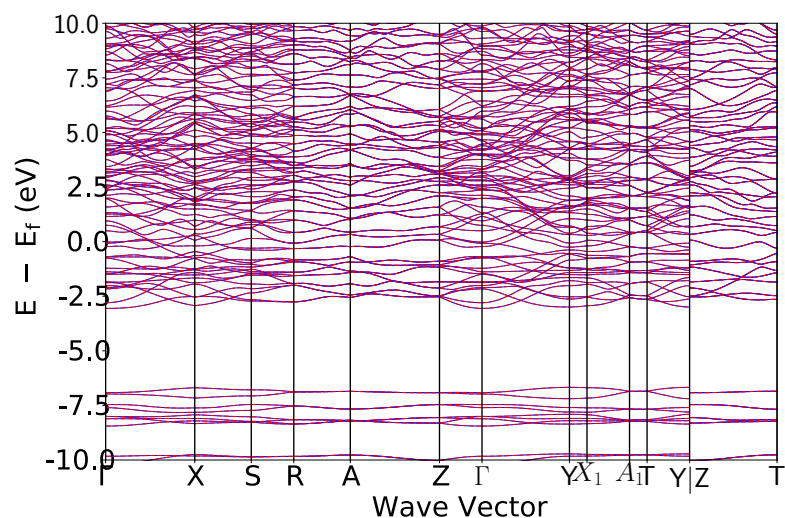


Figure 56: Ba_3Pb_5 (mp-630923). Symmetry: orthorhombic; Cmcm (number 63). Structure: Ba_3Pb_5 -type. Origin: ICSD;⁴¹ comments: “ Ba_3X_5 ($\text{X} = \text{Sn}, \text{Pb}$) and Sr_3Sn_5 fall into the region between the classical Zintl phases and intermetallic compounds”. Anionic electron coordination environment: linear with Ba.

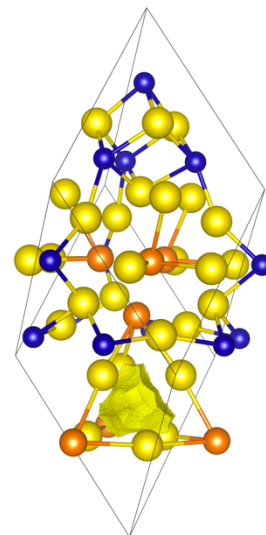
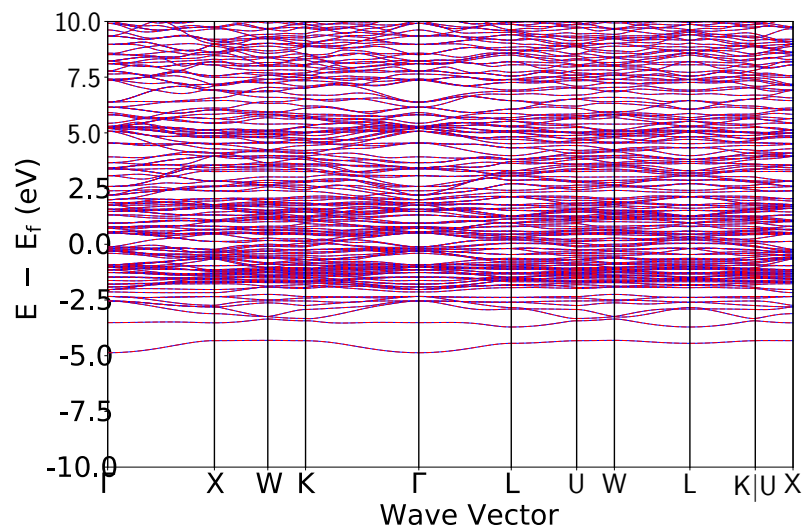


Figure 57: Pr_4MgCo (mp-645130). Symmetry: cubic; $F\bar{4}3m$ (number 216). Structure: NiTi_2 -type. Origin: ICSD;⁴² comments: referred to as intermetallic. Anionic electron coordination environment: octahedral with Pr.

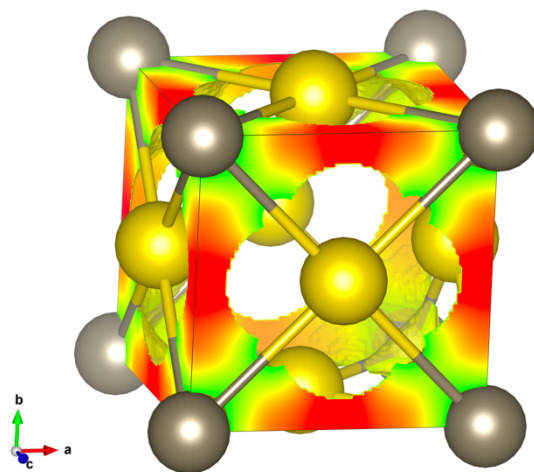
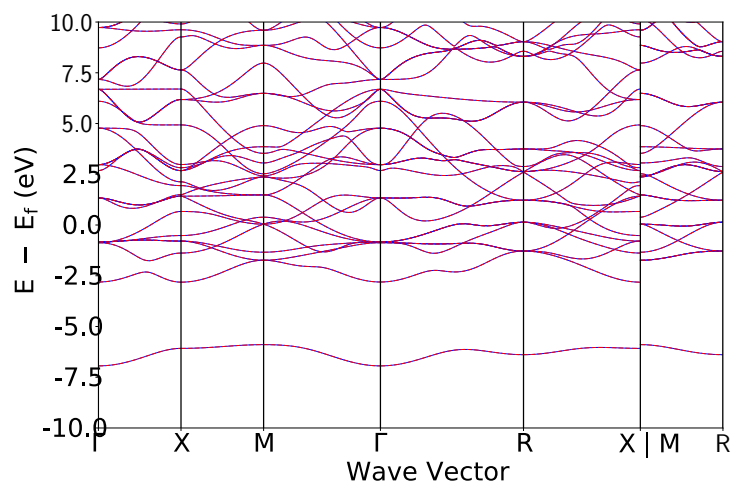


Figure 58: Pr_3Ti (mp-693). Symmetry: cubic; Pm-3m (number 221). Structure: Cu_3Au -type. Origin: ICSD;⁴³ comments: referred to as intermetallic. Anionic electron coordination environment: octahedral with Pr and Ti.

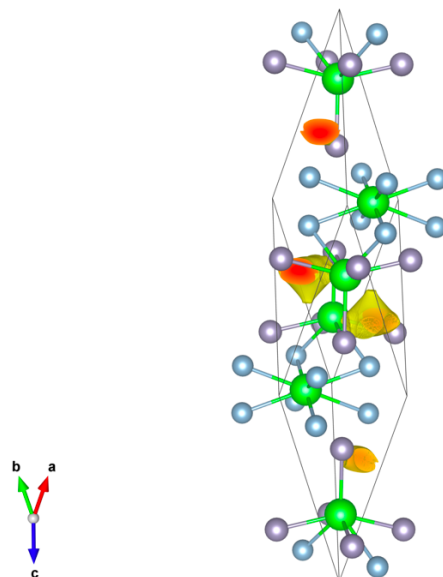
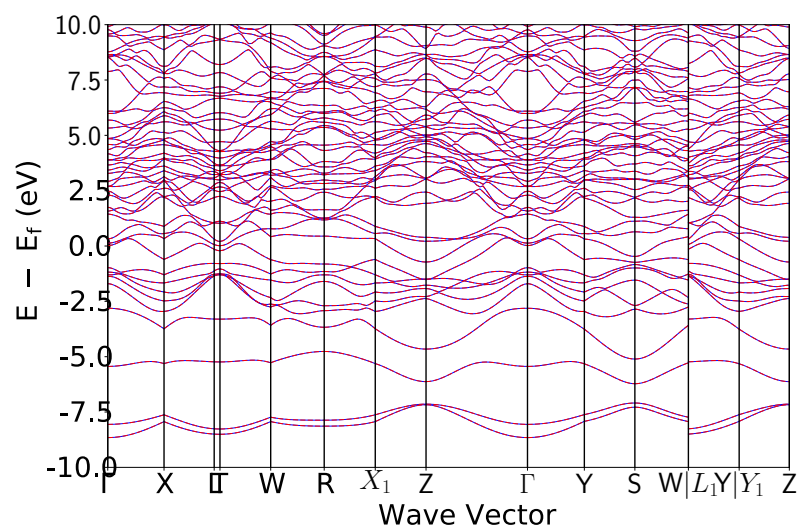


Figure 59: $\text{Sr}_3(\text{AlSn})_2$ (mp-7376). Symmetry: orthorhombic; Immm (number 71). Structure: Ta_3B_4 -type. Origin: ICSD;⁴⁴ comments: N/A. Anionic electron coordination environment: distorted square pyramidal with Sr, Al and Sn

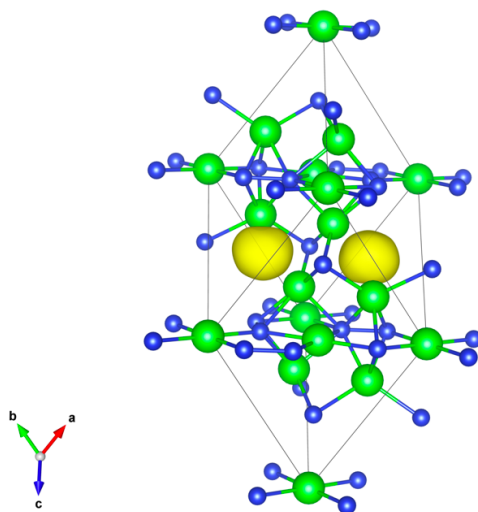
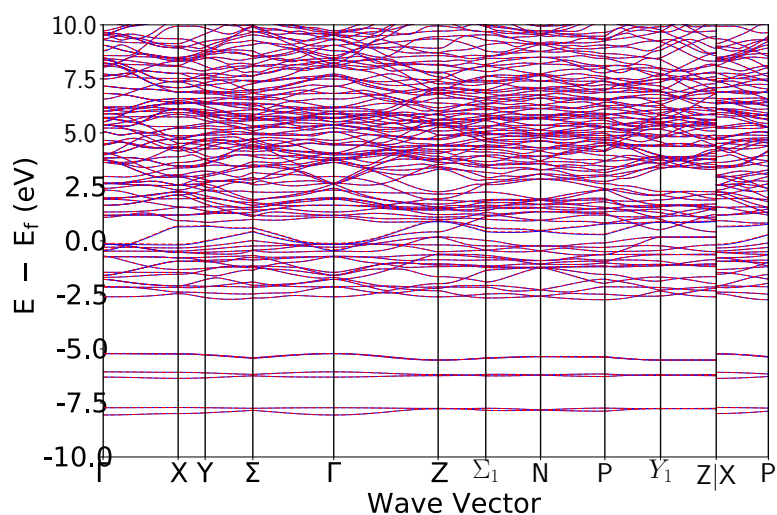


Figure 60: Sr_5Si_3 (mp-746). Symmetry: tetragonal; I4/mcm (number 140). Structure: Cr_5B_3 -type. Origin: ICSD;⁹ comments: *ab initio* predicted structure. Anionic electron coordination environment: tetrahedral with Sr.

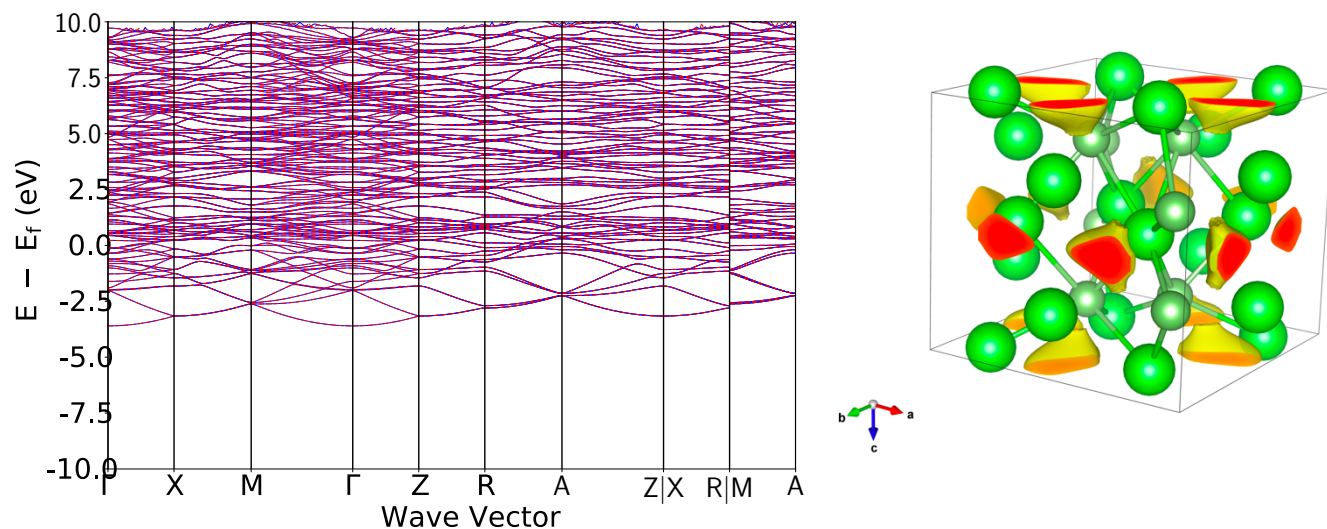


Figure 61: Sr_3Li_2 (mp-7507). Symmetry: tetragonal; $P4_2/mmm$ (number 136). Structure: Gd_3Al_2 -type. Origin: ICSD;⁴⁵ comment: referred to as intermetallic. Anionic electron coordination environment: square pyramidal with Sr and Li.

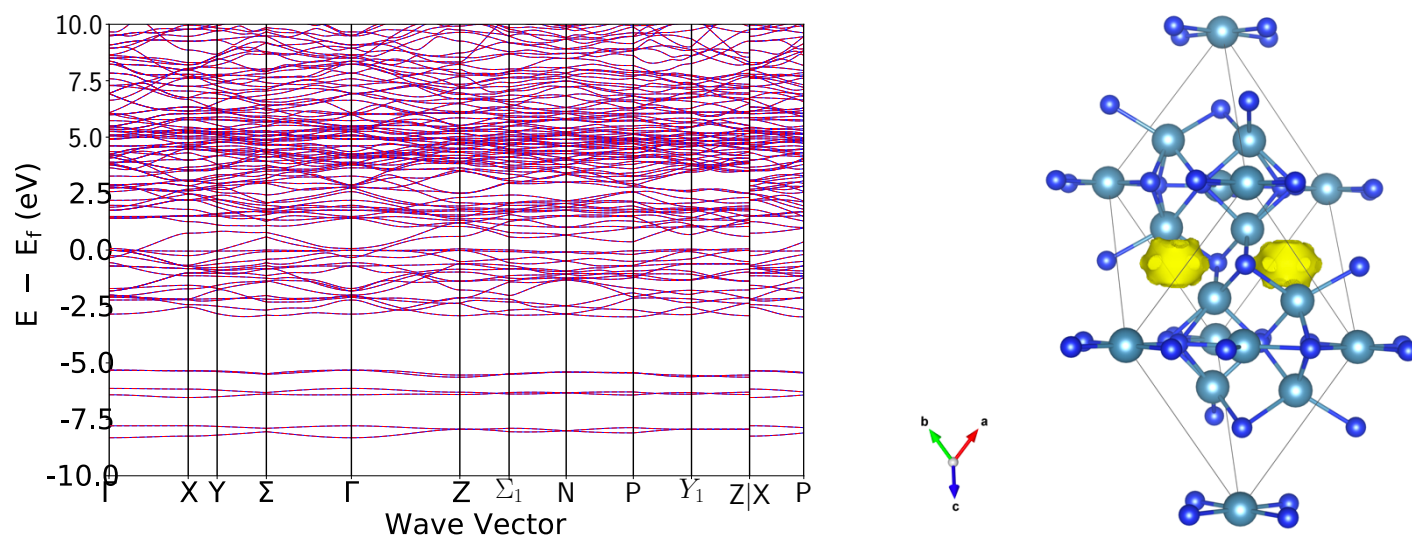


Figure 62: Ca_5Si_3 (mp-793). Symmetry: tetragonal; $I4/mcm$ (number 140). Structure: Cr_5B_3 -type. Origin: ICSD;²¹ comments: referred to as Zintl phase. Suggest unresolved hydrogen might be included in structure. Anionic electron coordination environment: tetrahedral with Ca.

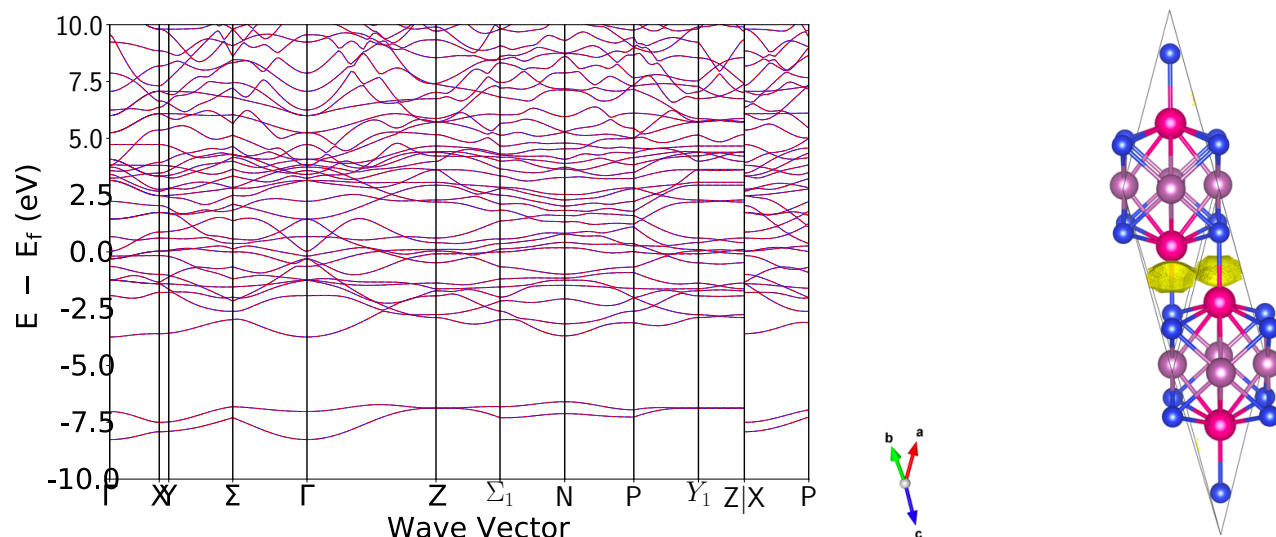


Figure 63: SmScSi (mp-8320). Symmetry: tetragonal; $I4/mmm$ (number 139). Structure: CeScSi -type. Origin: ICSD;⁴⁶ comments: N/A. Anionic electron coordination environment: tetrahedral with Sm.

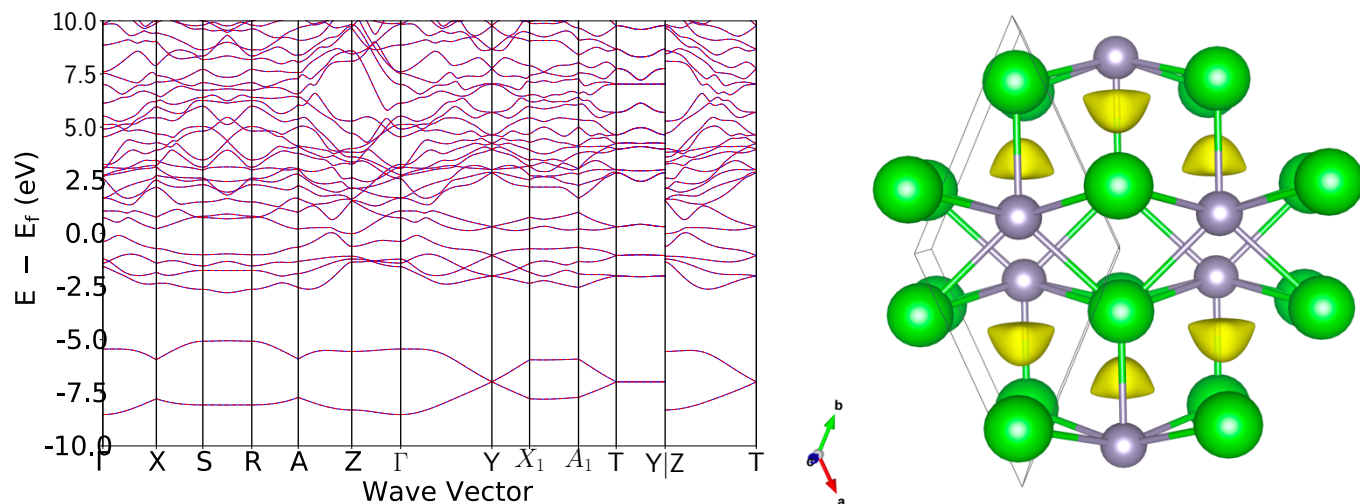


Figure 64: BaSn (mp-872). Symmetry: orthorhombic; Cmc₂m (number 63). Structure: CrB-type. Origin: ICSD; ¹⁶ comments: described as Zintl: “general valence equation suggests the presence of anion-anion chains”, reacts violently with moisture. Anionic electron coordination environment: distorted octahedral with Ba and Sn.

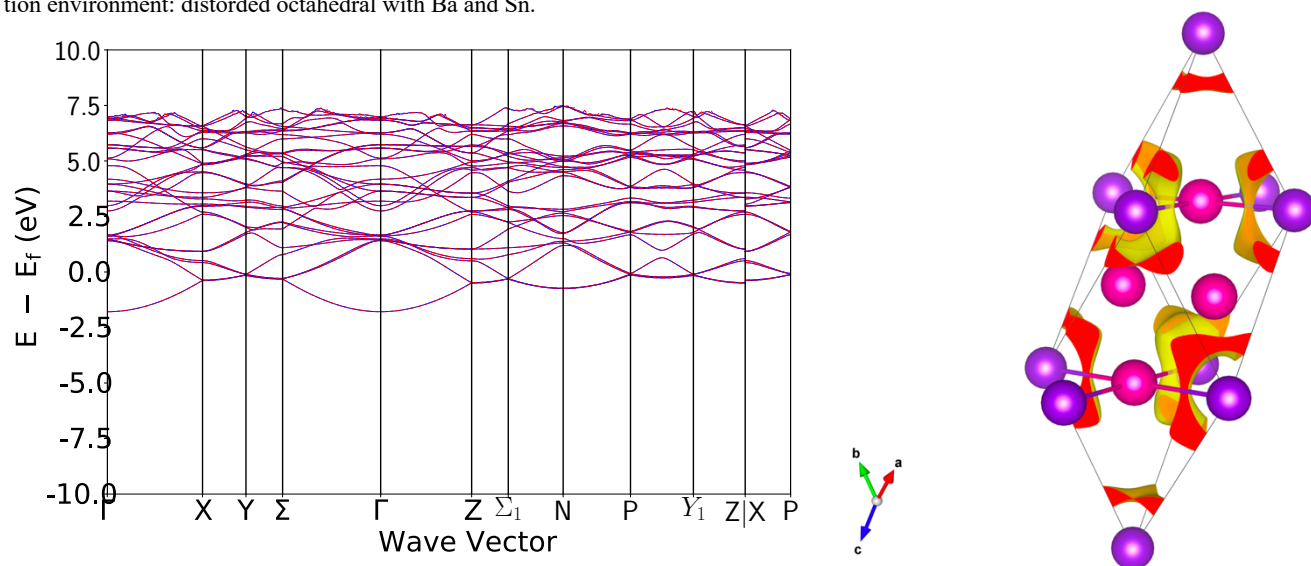


Figure 65: KRb₃ (mp-973508). Symmetry: tetragonal; I4/mmm (number 221). Structure: KRb₃-type. Origin: OQMD; ⁴⁷ comments: N/A. Anionic electron coordination environment: tetrahedral with K and Rb.

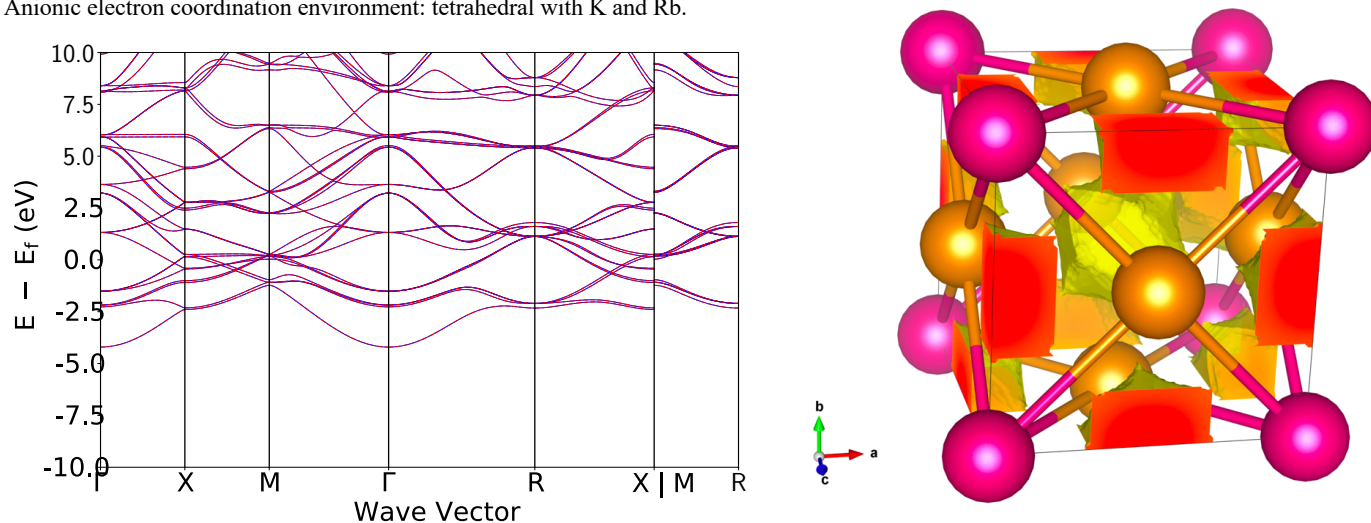


Figure 66: Nd₃Sm (mp-974066). Symmetry: cubic; Pm-3m (number 221). Structure: Cu₃Au-type. Origin: OQMD; ⁴⁷ comments: N/A. Anionic electron coordination environment: octahedral with Nd and Sm.

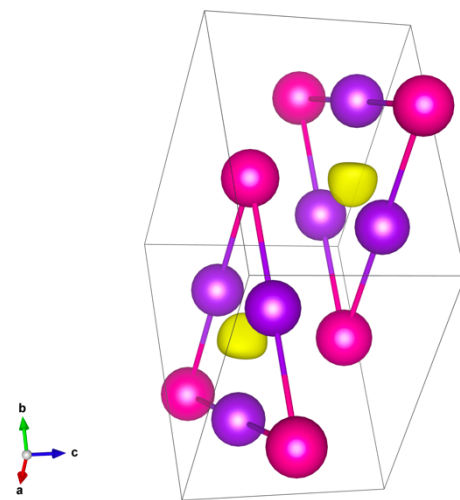
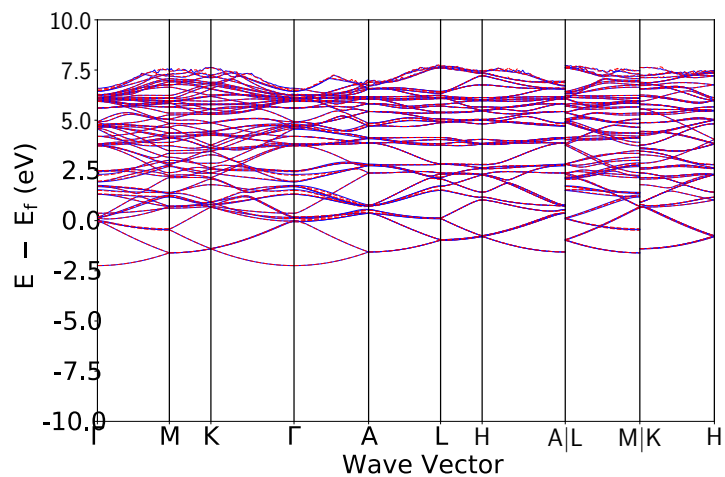


Figure 67: K_3Rb (mp-976115). Symmetry: hexagonal; $P6_3/mmc$ (number 194). Structure: HCP-metal. Origin: OQMD;⁴⁷ comments: N/A. Anionic electron coordination environment: trigonal planar with K.

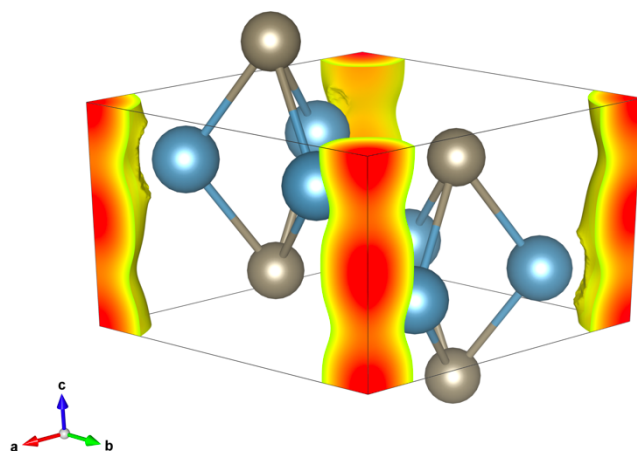
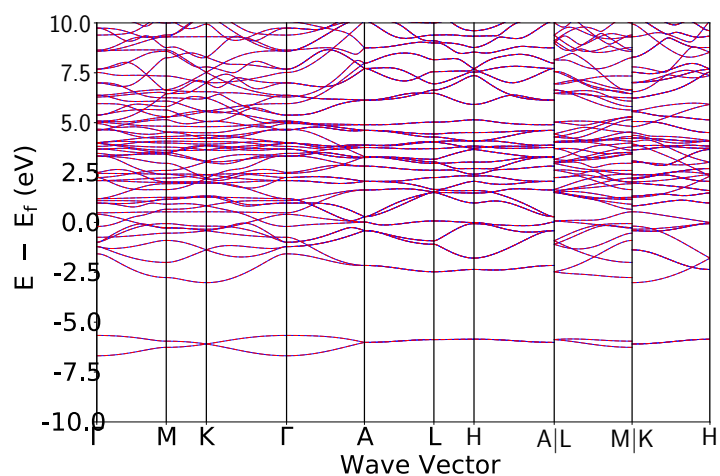


Figure 68: Ca_3Tl (mp-984744). Symmetry: hexagonal; $P6_3/mmc$ (number 194). Structure: HCP-metal. Origin: OQMD;⁴⁷ comments: N/A. Anionic electron coordination environment: octahedral with Ca.

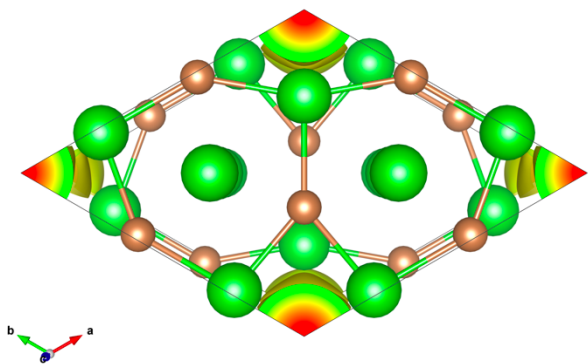
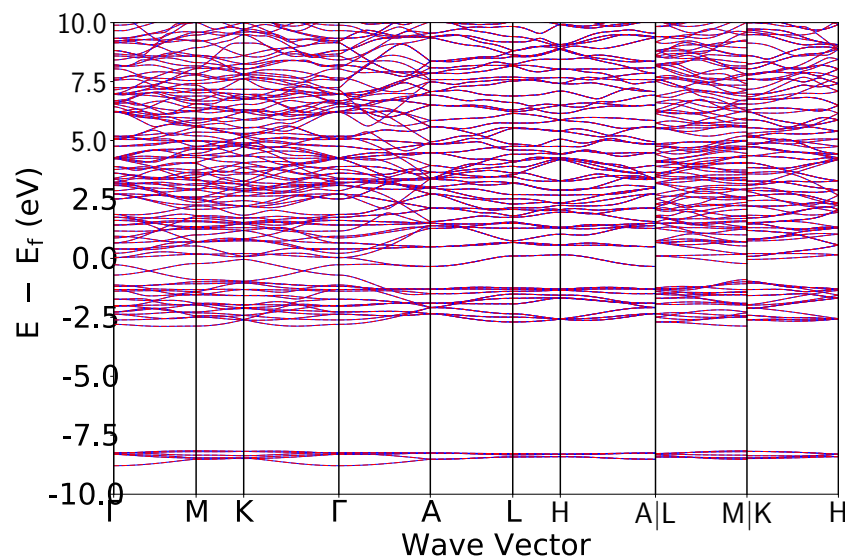


Figure 69: Ba_5Sb_3 (mp-9909). Symmetry: hexagonal; $P6_3/mcm$ (number 193). Structure: Mn_5Si_3 -type. Origin: ICSD;³¹ comments: N/A. Anionic electron coordination environment: octahedral with Ba.

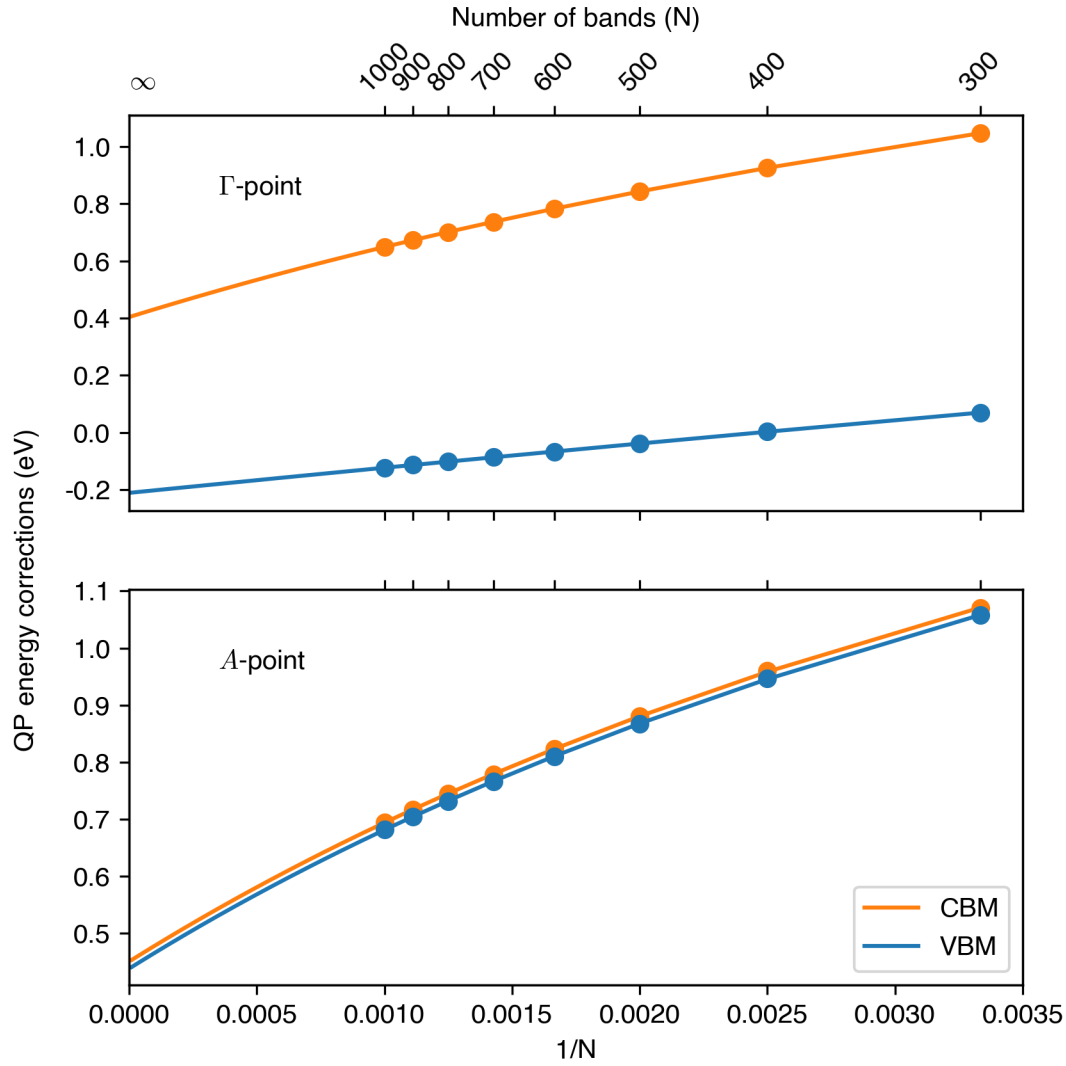


Figure 70: the convergence of quasi-particle energy corrections is plotted with respect to the number of bands included in the self-energy calculation for Sr_3CrN_3 . The quasi-particle corrections are obtained from the one-shot G0W0 calculations, and the convergence behaviour is expected to apply to self-consistent QSGW calculations. While the quasi-particle corrections are not fully converged even with 1000 bands, both the valence band maximum and conduction band minimum exhibit identical corrections at the A-point irrespective of the number of bands, essentially leaving the band gap closed even if the individual bands are less converged. The same convergence behaviour also applies to Ba_3CrN_3 .

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